SENES CONSULTANTS LIMITED

Specialists in Energy, Nuclear and Environmental Sciences

REACTIVE ACID TAILINGS ASSESSMENT PROGRAM (RATAP) USER'S MANUAL

A RESEARCH REPORT PREPARED UNDER
CONTRACT #23440-6-9196/01-SQ

FOR

ENERGY, MINES AND RESOURCES CANADA
CANADA CENTRE FOR MINERAL AND ENERGY TECHNOLOGY
MINERAL SCIENCES LABORATORIES
555 BOOTH STREET
OTTAWA, ONTARIO
K1A 0G1

BY

SENES CONSULTANTS LIMITED
499 McNICOLL AVENUE
WILLOWDALE, ONTARIO
M2H 2C9

March 1987

189 pp

MICROMEDIA

ABSTRACT

This publication is a user's manual for the Reactive Acid Tailings Assessment Program (RATAP), a probabilistic mathematical model which was developed to evaluate the rate and quantity of acid generated by the bacteria-assisted oxidation of sulfide minerals in uranium tailings. Background material on the model was documented as part of a previous study undertaken for the National Uranium Tailings Program. The model was developed to predict the long-term effects of Canadian uranium mill tailings although it is applicable to other sulphidic tailings.

The manual provides background information regarding the structure of RATAP and describes its input and output characteristics. RATAP consists of six components: initial inventory, kinetics, oxygen, pyrite oxidation, solute transport, and aqueous speciation. The information provided is sufficient to allow a user to run the program as it currently exists or modify the inputs to obtain a variety of outputs. Furthermore, sufficient details are provided to the user to modify existing modules of the code and/or replace entire modules.

NOTICE

This report was prepared by SENES Consultants Limited (SENES) under contract to the Canada Centre for Mineral and Energy Technology (CANMET). Neither CANMET nor SENES makes any warranty, expressed or implied, or assumes any liability with respect to any damage or loss incurred as a result of the use made of the information contained in this publication.

ABRÉGÉ

Le présent manuel s'adresse aux usagers du Programme d'évaluation des acides réactifs stériles (RATAP), modèle mathématique probabiliste qui a été conçu afin d'évaluer le taux et la quantité d'acide produit par l'oxydation de minéraux de sulfure, à l'aide de bactéries, dans des bassins d'uranium. Les données de base du modèle proviennent d'une étude précédente effectuée dans le cadre du Programme national de recherches sur les résidus d'uranium. Ce modèle a été mis au point afin de prévoir les effets à long terme des bassins d'uranium dans les usines au Canada, bien qu'il puisse s'appliquer à d'autres bassins sulfuriques.

Ce manuel donne l'information de base concernant la structure du RATAP. Il en décrit également les caractéristiques de départ et les effets. Le RATAP comporte six composants : le matériel de départ, la cinétique, l'oxygène, l'oxydation à la pyrite, le transport en solution et la spéciation aqueuse. Le manuel comprend suffisamment d'information pour permettre à un usager d'appliquer le programme tel qu'il existe ou de modifier les données de bases pour obtenir différents effets. Par ailleurs, l'usager trouvera les détails nécessaires à la modification de certaines sections du code, au remplacement d'une section, ou les deux.

TABLE OF CONTENTS

Page

Abstract i

Notice i

1.0 INTRODUCTION 1-1
- 1.1 Background 1-1
- 1.2 Concept of Probabilistic Analysis 1-2
- 1.3 How to Use the Manual 1-3
- 1.4 Objectives of RATAP 1-3
- 1.5 Input Parameters 1-4
- 1.6 Intermediate Parameters 1-4

2.0 CONTROL MODULES FUNCTIONS 2-1
- 2.1 Basic Functions 2-1
- 2.2. Draw Random Samples 2-1
- 2.3 Select Parameters for Output and Statistics 2-1
- 2.4 Compute Statistics on Selected Variables 2-2
- 2.5 Write Data to Output Files 2-2
  - 2.5.1 Statistics File 2-2
  - 2.5.2 Detailed Results File 2-2

3.0 BUILDING INPUT FILES AND OBTAINING OUTPUT 3-1
- 3.1 First Input File 3-1
  - 3.1.1 Input Arrays 3-2
  - 3.1.2 Model Portability 3-3
  - 3.1.3 Deterministic Runs 3-3
  - 3.1.4 Detailed Modular Output 3-3
- 3.2 Second Input File 3-4
  - 3.2.1 Maximum Output Array Size 3-4

Table of Contents, Cont'd.

Page

4.0 COMPILING AND LINKING 4-1

5.0 RUNNING THE PROGRAM 5-1
  5.1 Model Test 5-1

6.0 ALTERING THE PROGRAM 6-1
  6.1 Changing COMEX 6-1
  6.2 Writing Component Modules 6-2
  6.3 Passing Variables 6-2
    6.3.1 Include File MODEL.INC 6-3
    6.3.2 Include File INTERM INC 6-3
  6.4 Obtaining Additional Outputs 6-3
  6.5 Modifying First Input File 6-3
  6.6 Modifying Second Input File 6-3

REFERENCES

APPENDIX A - DESCRIPTION OF RATAP

A.1 Overview of RATAP
A.2 Initial Inventory Module
A.3 Kinetics Module
A.4 Oxygen Module
A.5 Pyrite Oxidation Module
A.6 Solute Transport Module
A.7 Speciation Module
A.8 References

Table of Contents, Cont'd.

Page

APPENDIX B - COMPUTER CODE
APPENDIX C - SAMPLE INPUT FILES
    C.1 Input P.dat
    C.2 Input D.dat
    C.3 Input 2.dat
APPENDIX D - SAMPLE OUTPUT FILES
    D.1 Probabilistic
    D.2 Deterministic
APPENDIX E - INPUT PARAMETER DESCRIPTIONS
APPENDIX F - INTERMEDIATE PARAMETERS
APPENDIX G - ERROR AND WARNING MESSAGES

LIST OF FIGURES

		Follows Page
1.1	Concept of Probabilistic Analyses	1-2
3.1	Input and Output Files	3-1
3.2	Forms of the Weibull Distribution Probability Function	3-2
3.3	Forms of the Beta Distribution Probability Density Function	3-2
3.4	An Arbitrary Probability Density Function	3-2
6.1	System Model	6-1
6.2	Control Module Structure	6-1
6.3	Subroutine Comex and the Component Modules	6-1
A.1	Concept Adopted for Modelling of Tailings	A-1
A.2	Conceptual Flow Diagram	A-2
A.3	pH Computational Scenarios	A-3

LIST OF TABLES

	Follows Page
3.1. Sample of First Input File	3-1
3.2 Format of First Input File	3-1
3.3 Distribution Descriptors	3-2
3.4 Sample of Second Input File (INPUT2.DAT)	3-4
3.5 Format of Second Input File	3-4
5.1 Sample Session	5-1

1.0 INTRODUCTION

1.1 Background

In 1982 Energy, Mines and Resources Canada established the National Uranium Tailings Program (NUTP) to conduct research into the long-term environmental behaviour of uranium mill tailings. The main objective of the NUTP was to provide a scientifically credible information base for use in developing the capability to predict the long-term effects of uranium tailings with a known degree of confidence while incorporating variability and uncertainty in the input data.

The emphasis in the research program supported by the NUTP was the development of a probabilistic assessment tool for predicting the release rate of contaminants from tailings piles and simulating their transport through the environment to humans (SENES, 1984, 1985, 1986, 1987a). In another research investigation supported by the NUTP, particular attention was given to understanding the geochemical processes which control the evolution of both sulphidic uranium tailings, typical of those found in northern Ontario (SENES and Beak, 1986). These investigations considered physical, chemical, and biological factors at a very complex, precise scale of investigation.

The stated objective of this research work was to develop a user's manual for the Reactive Acid Tailings Assessment Program (RATAP). RATAP provides an estimate of the upper and lower limits of the rate and quantity of acid generation by the bacteria-assisted oxidation of pyrite and other sulfide minerals present in uranium mill tailings, and is fully documented in a previous report (SENES and Beak, 1986).

The RATAP model is based upon principles of mass balance and employs geochemical kinetics or equilibria where appropriate and solution transport to estimate the pH and the acidity of porewater. A probabilistic technique is used to analyze the effects of oxidation processes and variables on the rate and quantity of acid generation. The model employs algorithms derived from theoretical and experimental considerations.

1.2 The Concept of Probilistic Analysis

As with any predictive assessment, probilistic analysis involves a mathematical expression (model) of some physical system, in this case a uranium tailings. The model is a mathematical expression to which information is supplied in the form of numerical values for one or more input variables and it produces the corresponding numerical values of one or more output variables.

Most of the input variables required by such a model are not known with certainty. The uncertainty arises because of normal experimental error in their measurement or because (sometimes) actual measurements are impossible and judgement must be used. Consequently, it is impossible for most input variables to be adequately characterized by any single number. Fortunately, our full state of knowledge about any input variable can be described in the form of a (subjective) probability distribution.

Having specified the input distributions it is necessary to determine the corresponding values of the output variables. Because many of the input parameters are specified as distributions, rather than as single numbers, distributions, rather than single numbers will be obtained for the calculated variables. The distribution of calculated results is obtained by using a statistical sampling or Monte Carlo procedure which involves drawing many samples from each input parameter distribution. The procedure, illustrated in Figure 1.1, is a repetitive one. At each repetition a single value is drawn for each input variable from its probability distribution. These values of the input variables are substituted into the mathematical model (the component models) to obtain a single value for each output variable. This process, which is referred to as a trial, is then repeated as often as desired.

The output variable(s) from such an analysis can be considered as a sample(s) on an objective random variable(s) corresponding to that output variable(s).

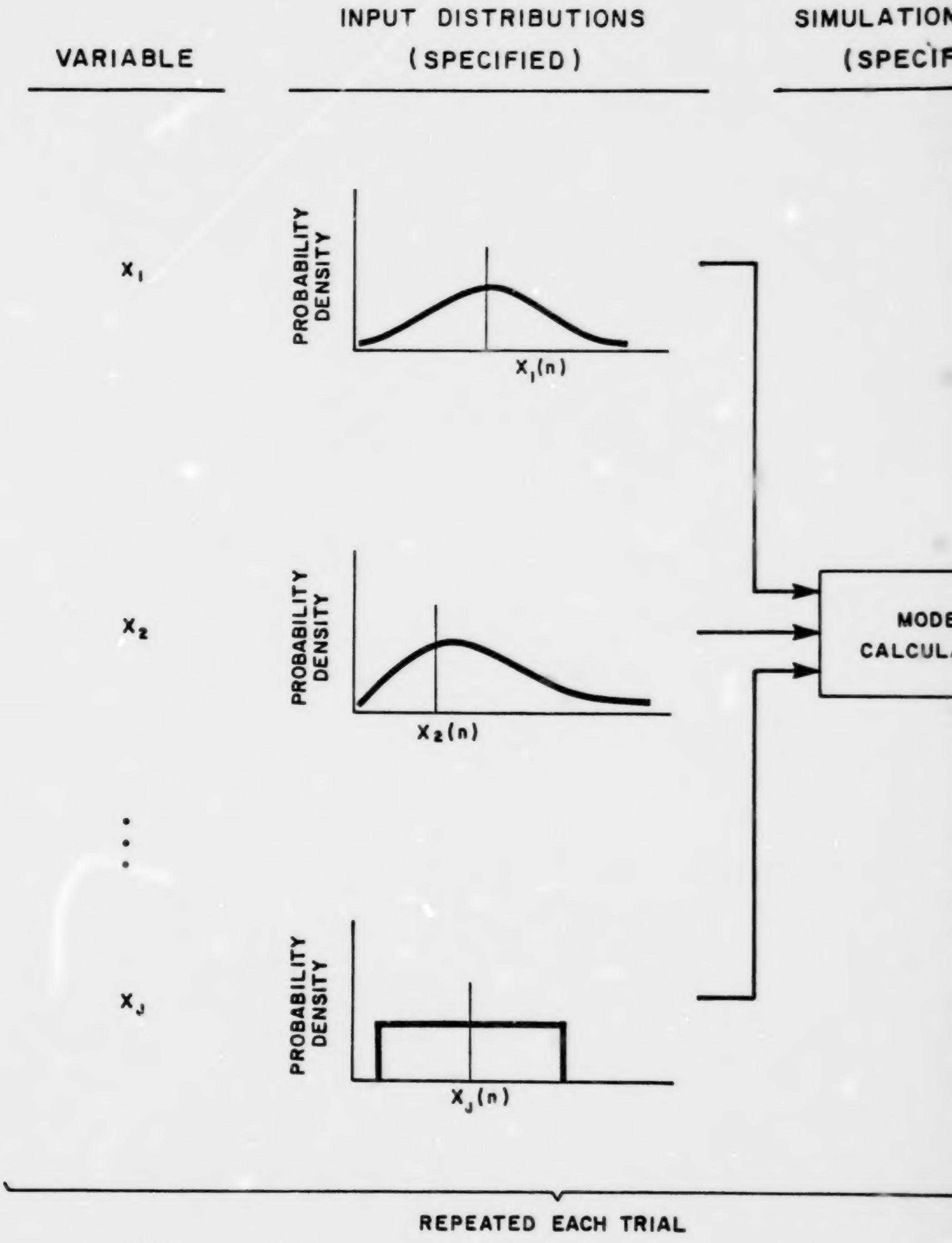
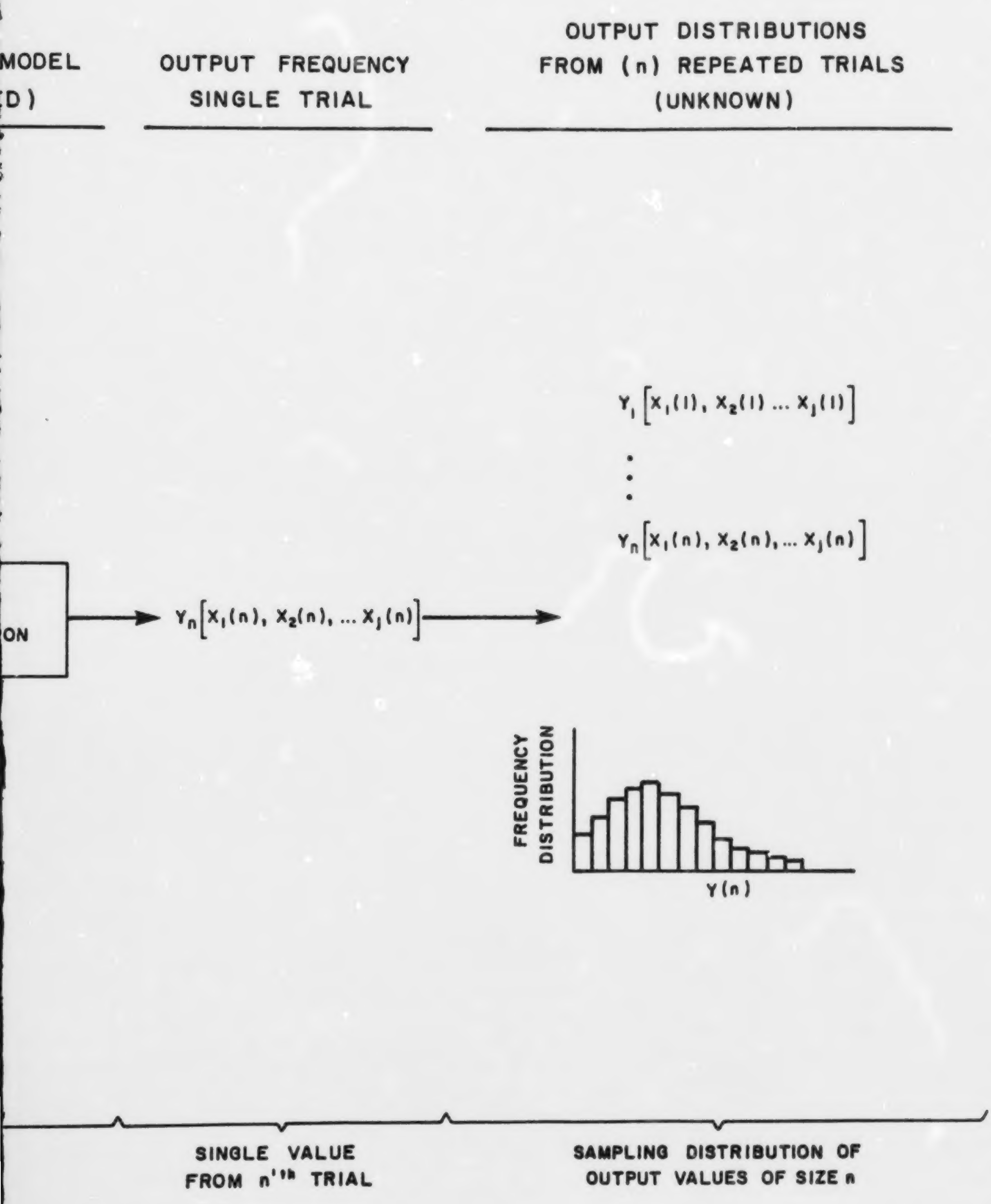

VARIABLE
INPUT DISTRIBUTIONS
(SPECIFIED)
SIMULATION
(SPECIF
X_1
PROBABILITY DENSITY
$X_1(n)$
X_2
PROBABILITY DENSITY
$X_2(n)$
X_J
PROBABILITY DENSITY
$X_J(n)$
MODE
CALCUL
REPEATED EACH TRIAL

FIGURE 1.1

CONCEPT OF PROBABILISTIC ANALYSIS


MODEL
OUTPUT FREQUENCY
SINGLE TRIAL
OUTPUT DISTRIBUTIONS
FROM (n) REPEATED TRIALS
(UNKNOWN)
$Y_1[X_1(1), X_2(1) \dots X_j(1)]$
$Y_n[X_1(n), X_2(n), \dots X_j(n)]$
ON
$Y_n[X_1(n), X_2(n), \dots X_j(n)]$
FREQUENCY
DISTRIBUTION
Y(n)
SINGLE VALUE
FROM n'th TRIAL
SAMPLING DISTRIBUTION OF
OUTPUT VALUES OF SIZE n

From the sample, the mean, variance, probability density function (pdf) or cumulative distribution function (cdf) may be estimated as desired. This information may be interpreted as describing the output variable in terms of subjective probability; telling us quantitatively what we are entitled to believe about the output variable.

1.3 How to Use the Manual

The user's manual for RATAP is geared toward two types of users. The first type is the Level I user who simply wishes to use the program. Such considerations as building and modifying input files and obtaining desired output are dealt with in the first five chapters. The second type of user is the Level II user who actually wishes to change the program by adding new lines of code or new modules. The level of detail provided to the Level II user is, hence, considerably higher.

The first five chapters of this manual provide both Level I and II users with necessary background to build input files, compile, link and run the program. The sixth chapter, titled "Altering the Program", is intended for the Level II user. The appendices provide a description of RATAP, the computer code, sample input and output files and error and warning messages.

1.4 Objectives of RATAP

The principal objective of the Reactive Acid Tailings Assessment Program is to perform a probabilistic analysis of the rate and quantity of acid generated by bacteria-assisted oxidation of pyrite and other sulfide minerals. The model has been designed to allow predictions of monthly, yearly and cumulative acid flux from a tailings site.

In addition the model provides many other features. These include the ability to incorporate up to twenty-two distinct soil layers, i.e. each layer has unique soil parameter values. This feature allows the user to specify the characteristics of various types of cover materials for use in analysing close-out options.

1.5 Input Parameters

One of the advantages of RATAP is that it is non-site specific. This portability is achieved by allowing the user to specify input values for all important model parameters. A complete list of input parameters is given in Appendix E. The user can change the inputs to model a particular tailings site or to develop and test a particular scenario. This feature is expanded upon in Section 3.1.

1.6 Intermediate Parameters

In order to estimate the upper and lower limits of the rate and quantity of acid generated, several intermediate parameters are calculated. These include: soil temperature, soil water content, rates of chemical and biological oxidation, gaseous phase concentration of oxygen profiles, aqueous phase concentrations of aluminum, calcium, sulfate, iron, hydronium ion, carbonate, and solid phase concentrations of calcite, gypsum, aluminum hydroxide and ferric hydroxide. A list of the intermediate parameters is presented in Appendix F.

2.0 CONTROL MODULES FUNCTIONS

2.1 Basic Functions

The control modules open, access and read all of the input files. They draw random samples for the parameters with specified distribution and route the parameter values to the appropriate component modules. The control modules adjust the time as well as store selected parameters for output. The final task of the modules is to compute statistics on selected parameter for ouput. The final task of the modules is to compute statistics on selected variables and write this data to output files.

2.2 Draw Random Samples

The control modules have the capability of drawing random samples from the following user-specified probability distributions for input model parameters:

1) Constant
2) Normal
3) Lognormal
4) Uniform
5) Log-uniform
6) Triangular
7) Weibull
8) Beta
9) Arbitrary
10) Correlated

Variables are sampled once for each trial except for those specified as time-variant which are sampled each time step of each trial.

The selected random samples are routed to the appropriate component modules.

2.3 Select Parameters for Output and Statistics

The user may specify calculated variables as well as selected input parameters for output at selected time intervals without having to alter the program. These data reside in a series of arrays in the program. Parameter selection for output is achieved by specifying the time intervals desired and the position in the output variable arrays(eg. layer number) required for output.

Two output options are available: 1) summary statistics (called the key file) or 2) summary satistics (key file) and a detailed ouput of selected parameters for all trials (called the res file).

Detailed modular output is also possible. The selection of the particular modular output required is performed in the first input file. A detailed discussion of this ouput is presented in Section 3.1.4.

2.4 Compute Statistics on Selected Variables

Summary statistics are computed for user-selected output parameters and input distributions. These statistics are updated at the end of each trial and printed to a disk file at the end of the simulation.

2.5 Write Data to Output Files

The two output files discussed below are available to the user. Sample output files are shown in Appendix D.

2.5.1 Statistics File (Key File)

This file is the default and is created for every run. The following summary statistics computed by the statistics routines are output to a user-specified disk file, called key file:

Mean
Standard deviation
Geometric mean
Geometric standard deviation
Minimum
Maximum

Skewness and Kurtosis can also be printed to the key file as an option.

The parameter names, specifications, and the time intervals selected are also output, as appropriate.

Statistics not calculated will appear as blanks in the key file. For instance, if only one trial is performed, standard deviations, skewness and kurtosis will not be calculated and blanks will appear for these in the key file.

2.5.2 Detailed Results File (Res File)

The detailed results file can be selected in the first input file. The detailed results file contains the actual data from which the statistics written to the key file are calculated. The user-selected parameters are written to the detailed results file at the end of each trial. The rows of the key file correspond to the columns of the detailed results file. For instance, the third row of the key file describes the data contained in the third column of the detailed results file.

3.0 BUILDING INPUT FILES AND OBTAINING OUTPUT

In order to run RATAP, two input files are required. The first input file contains the probabilistic distributions or deterministic values of the various input parameters. The second file contains information on the selection of output parameters. The contents of the input files are illustrated in Figure 3.1. The user is prompted interactively for the names of the input files.

Listings of these two files are shown in Appendix C and the output files resulting from them are shown in Appendix D.

3.1 First Input File (INPUTP.DAT or INPUTD.DAT)

This file is used to specify the input parameters, and their distributions. Two types of input files can be selected. These are 1) a probabilistic file (INPUTP.DAT) or 2) a deterministic file (INPUTD.DAT). The remaining part of the discussion will be devoted to the probabilistic input set. A short description of the deterministic inputs is presented in Section 3.1.3. A sample probabilistic file is shown in Table 3.1. The descriptive labels present in Table 3.1, do not appear in the actual file. The format of this input file is given in Table 3.2.

The first line of the file is the title to be written to the statistics file. Next, the desired output files are specified and named. The user can specify: 1) a statistics (key file) or, 2) a detailed results (res file) and a statics file as described previously in Section 2.5.

The specifics of the run are set up by reading the random number seed, the number of trials, and the simulation time in months. The RATAP program uses a time increment of one month. The following random number seeds have been thoroughly tested:

824064364
913566091
2096730329
281629770

FIGURE 3.1

INPUT AND OUTPUT FILES

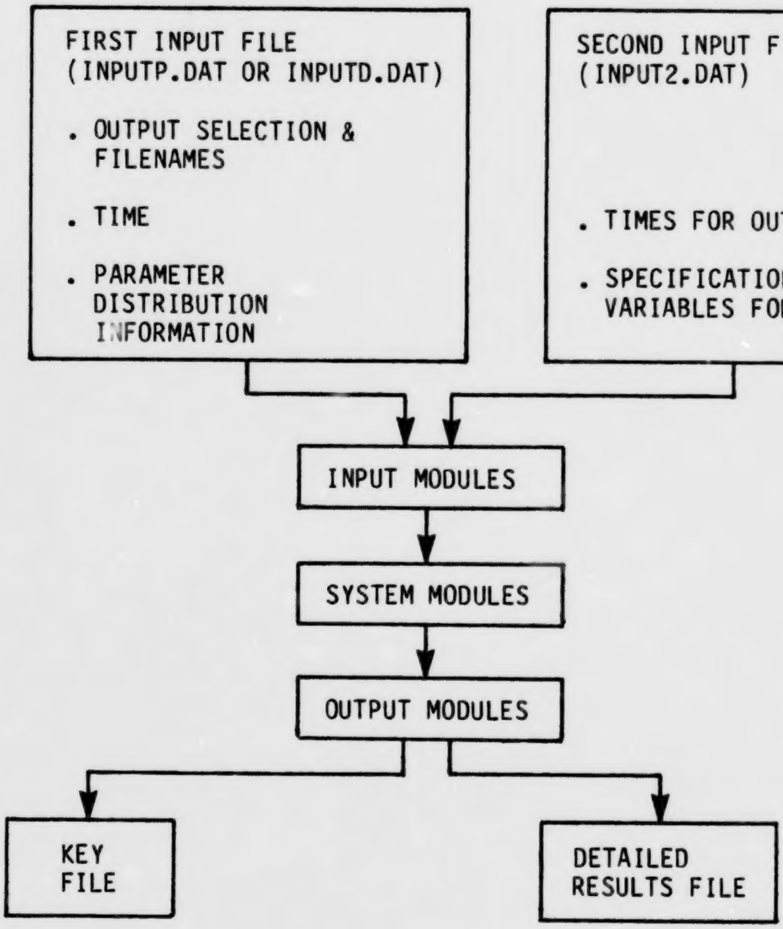

FIRST INPUT FILE
(INPUTP.DAT OR INPUTD.DAT)
. OUTPUT SELECTION & FILENAMES
. TIME
. PARAMETER DISTRIBUTION INFORMATION
SECOND INPUT FILE
(INPUT2.DAT)
. TIMES FOR OUTPUT
. SPECIFICATION OF VARIABLES FOR OUTPUT
INPUT MODULES
SYSTEM MODULES
OUTPUT MODULES
KEY FILE
DETAILED RESULTS FILE

Table 3.1

SAMPLE OF FIRST INPUT FILE

```
     Title
PROBABILISTIC ANALYSIS: TEST CASE

┌────Detailed Results file indicator
│ ┌───────Skewness and kurtosis indicator
N Y

     Detailed Results file name
RES.PRB
     Key file name
KEY.PRB
   ┌─Number of input distributions
   │   ┌───Number of arbitrary distributions
   │   │   ┌───Number of correlated parameters
  17   1   1
   ┌─Random number seed
   │         ┌───Number of trials
0913566091  50
    ┌─────Months in simulation
   186
     Module output control:

   ┌───────────Module output flag name
   │   ┌───────────Output flag
   │   │  ┌──────────────Distribution type number
   │   │  │ ┌──────────────Time-variant flag
   │   │  │ │        ┌─────────Flag value
FLAG1  N  1 N        1
FLAG2  N  1 N        1
FLAG3  N  1 N        1
FLAG4  N  1 N        1
FLAG5  N  1 N        1
FLAG6  N  1 N        1
     Month for detailed module output:

   ┌───────────Flag name
   │   ┌───────────Output flag
   │   │  ┌──────────────Distribution type number
   │   │  │ ┌──────────────Time-variant flag
   │   │  │ │        ┌─────────Month value
MONTH  N  1 N        6.
     Regular distributions:
   ┌──────Parameter name
   │   ┌──────Output flag
   │   │  ┌─────────Distribution type number
   │   │  │  ┌─────────Time-variant flag
   │   │  │  │               Distribution descriptors
CONST  N  1  N     2.0
NORMAL N  2  V    10.0       2.0          0.0         20.0
LNORM  N  3  V   1.0E02      1.5          1.0         1.0E3
UNI    F  4  N     1.0       2.0
LOGUNI N  5  N    0.01       0.5
TRIANG N  6  N    0.01       0.03         0.1
WEIBUL F  7  V     0.0       1.5          0.9
BETA   N  8  N    10.0     100.0          2.0          2.0
```

Arbitrary distributions:

```
             Parameter name
                  Output flag
                       Distribution type number
                            Time-variant flag
                                 Number of cells in distribution
                                      Distribution descriptors
ARB     N  9  N  10  1.0  11.0  2.0  2.0   2.0  8.0  8.0  8.0 12.0 12.0 4.0 4.0
```

Correlated distributions:

```
             Parameter name
                  Output flag
                       Distribution type number
                            Time-variant flag
                                 Name of independent distribution
                                      Distribution descriptors
CORREL N 10 N NORMAL      50.0       10.0       0.7       10.0        2.0
```

Table 3.2

FORMAT OF FIRST INPUT FILE

	Column	Format	Description
Line 1:	1-40	A40	Title
Line 2:	1	A1	Detailed results file desired (Y/N)
	3	A1	Skewness and Kurtosis desired in key file (Y/N)
Line 3:	1-12	A12	Detailed results file name
Line 4:	1-12	A12	Key file name
Line 5:	1-4	I4	Number of input distributions (max. 300)
	5-8	I4	Number of arbitrary distributions
	9-12	I4	Number of correlated parameters
Line 6:	1-10	I10	Random number seed
	11-14	I4	Number of trials
Line 7:	1-7	E7.2	Months in Simulation
Line 8-13:	1-6	A6	Detailed modular output flag name
	8	A1	Output flag (F/N)**
	10-11	I2	Distribution type number (Table 3.3)
	13	A1	Time variant flag (Variant, Not =>V/N*)
	14-25	E11.6	Detailed modular output (Yes, No =>1./0.)
Line 14:	1-6	A6	Month for detailed modular output, flag name
	8	A1	Output flag (F/N)**
	10-11	I2	Distribution type number (Table 3.3)
	13	A1	Time variant flag (Variant, Not =>V/N*)
	14-25	E11.6	Month for detailed modular output (1.=>12.)

Regular Distributions:

Constant, Normal, Lognormal, Uniform, Loguniform, Triangular, Weibull, and Beta distributions. One line for each distribution:

1-6	A6	Parameter name
8	A1	Output flag (F/N)**
10-11	I2	Distribution Type Number (Table 3.3)
13	A1	Time-Variant Flag (Variant, Not => V/N*)
14-57	4E11.6	Distribution Descriptions

Table 3.2/cont'd.

Arbitrary distributions. One line for each distribution:

1-6	A6	Parameter name
8	A1	Output flag (F/N)**
10-11	I2	Distribution Type Number (Table 3.3)
13	A1	Time-Variant Flag (Variant, Not =>V/N*)
14-16	I3	Number of cells in distribution (max. 25)
17-38	2E11.6	Minimum and Maximum value ordinates
39-188	25F6.2	Function value for each cell

Correlated distributions. One line for each distribution:

1-6	A6	Parameter name
8	A1	Output flag (F/N)**
10-11	I2	Distribution Type Number (Table 3.3)
13	A1	Time-Variant Flag (Variant, Not => V/N*)
15-20	A6	Name of independent variable
21-75	5E11.6	Distribution Descriptions

Notes
* V = time variant, N = non-time variant. Default is N, non-time variant.
**F = output to open files, N = no output of variable. Default is N, no output.

The input parameters are specified as distributions with their type numbers according to Table 3.3. Each type of distribution is specified using the appropriate distribution descriptor as indicated on Table 3.3 The Weibull, beta, and arbitrary distributions are illustrated in Figures 3.2, 3.3 and 3.4, respectively. The location parameter (a) for the Weibull distribution, not shown on Figure 3.2, determines the position of the origin on the horizontal axis. For instance, if a = 2 the origin is shifted from 0 to 2 on the horizontal axis.

The input paramters for which distributions must be specified are described in Appendix E. These must be entered in the same order as they appear in the appendix and in the example file, INPUTP.DAT, shown in Appendix C.

The "output flag" indicated in Table 3.2 (column 8) allows the user to output sampled parameter values to the openned statistics (key file) or detailed results (res file) files, if desired. The default is no output.

Distributions can be either time-variant or non-time-variant as indicated by the time-variant flag. The default is non-time-variant. Time-variant parameters are sampled for each time step of each trial while non-time-variant parameters are sampled once for each trial.

3.1.1 Input Arrays

In RATAP, the tailings soil profile is subdivided into a maximum of 22 distinct layers: one to twenty layers in the unsaturated zone and capillary fringe and one to two layers in the saturated zone. In order to incorporate the flexibility of layer selection, the control module has been programmed to read all twenty-two layers. Hence, for each layer dependent parameter twenty-two input values are present in the input files (see Appendix C). Therefore, the user must specify parameter values for each layer under study and assign a value of zero for each of the remaining layers.

Table 3.3

DISTRIBUTION DESCRIPTORS

Distribution	Distribution Number	Distribution Descriptors	Column
Constant	1	Constant	14-24
Normal	2	Mean	14-24
		Standard Deviation	25-35
		Minimum	36-46
		Maximum	47-57
Lognormal	3	Geometric Mean	14-24
		Geometric Standard Deviation	25-35
		Minimum	36-46
		Maximum	47-57
Uniform	4	Minimum	14-24
		Maximum	25-35
Log-uniform	5	Minimum	14-24
		Maximum	25-35
Triangular	6	Minimum	14-24
		Mode	25-35
		Maximum	36-46
Weibull (Figure 3.2)	7	Location Parameter (Minimum)(a)	14-24
		Scale Parameter (b)	25-35
		Shape Parameter (c)	36-46
Beta (Figure 3.3)	8	Minimum	14-24
		Maximum	25-35
		Shape Parameter (a)	36-46
		Shape Parameter (b)	47-57
Arbitrary (Figure 3.4)	9	Number of cells (max. 25)	14-16
		Minimum	17-27
		Maximum	28-38
		Ordinate Values	39-(188)
Correlated	10	Mean of dependent variable	21-31
		Standard Deviation of Dependent Variable	32-42
		Correlation Coefficient	43-53
		Mean of Independent Variable	54-64
		Standard Deviation of Independent Variable	65-75

FIGURE 3.2

FORMS OF THE WEIBULL DISTRIBUTION PROBABILITY DENSITY FUNCTION

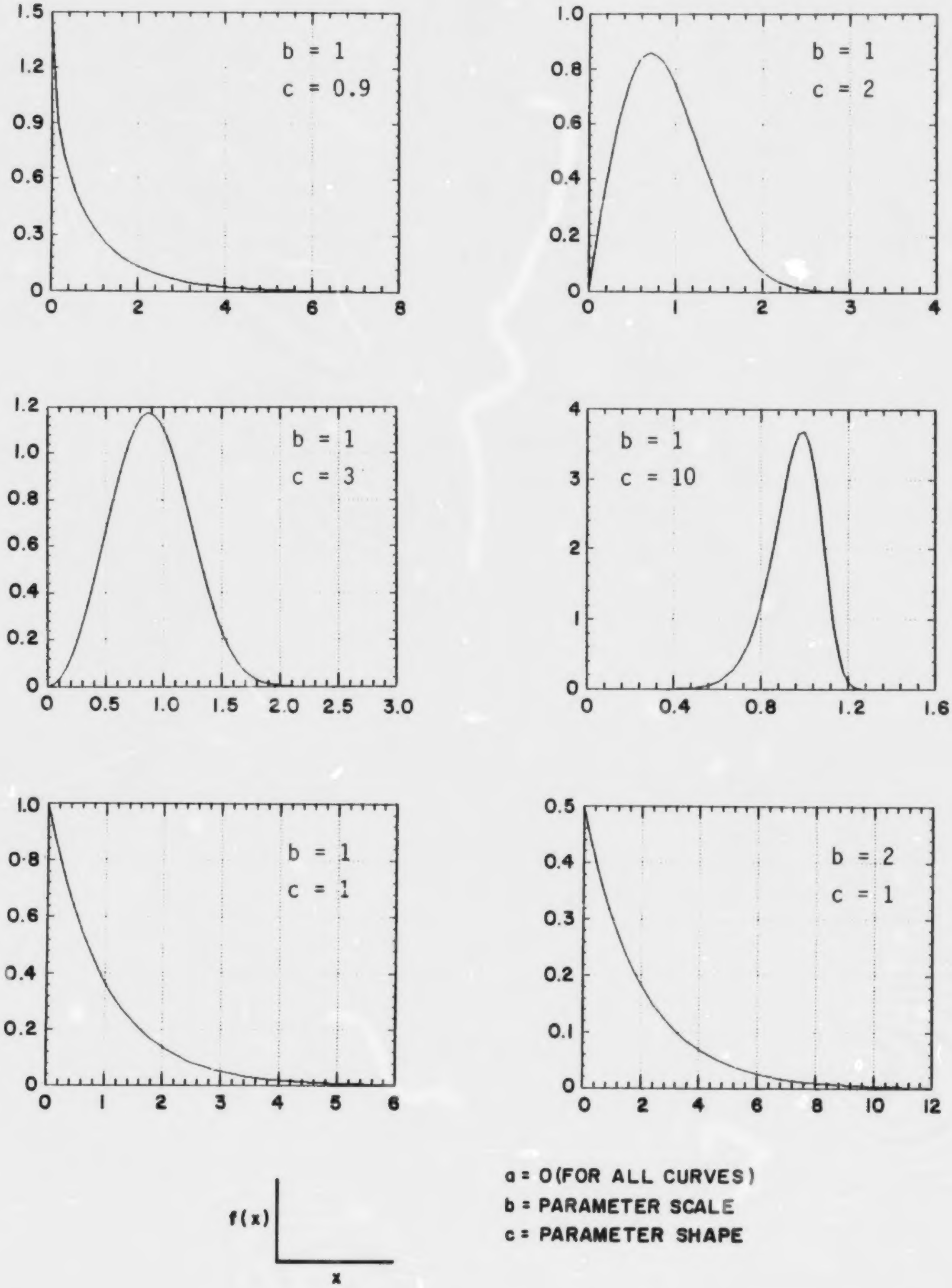


FIGURE 3.3

FORMS OF THE BETA DISTRIBUTION
PROBABILITY DENSITY FUNCTION

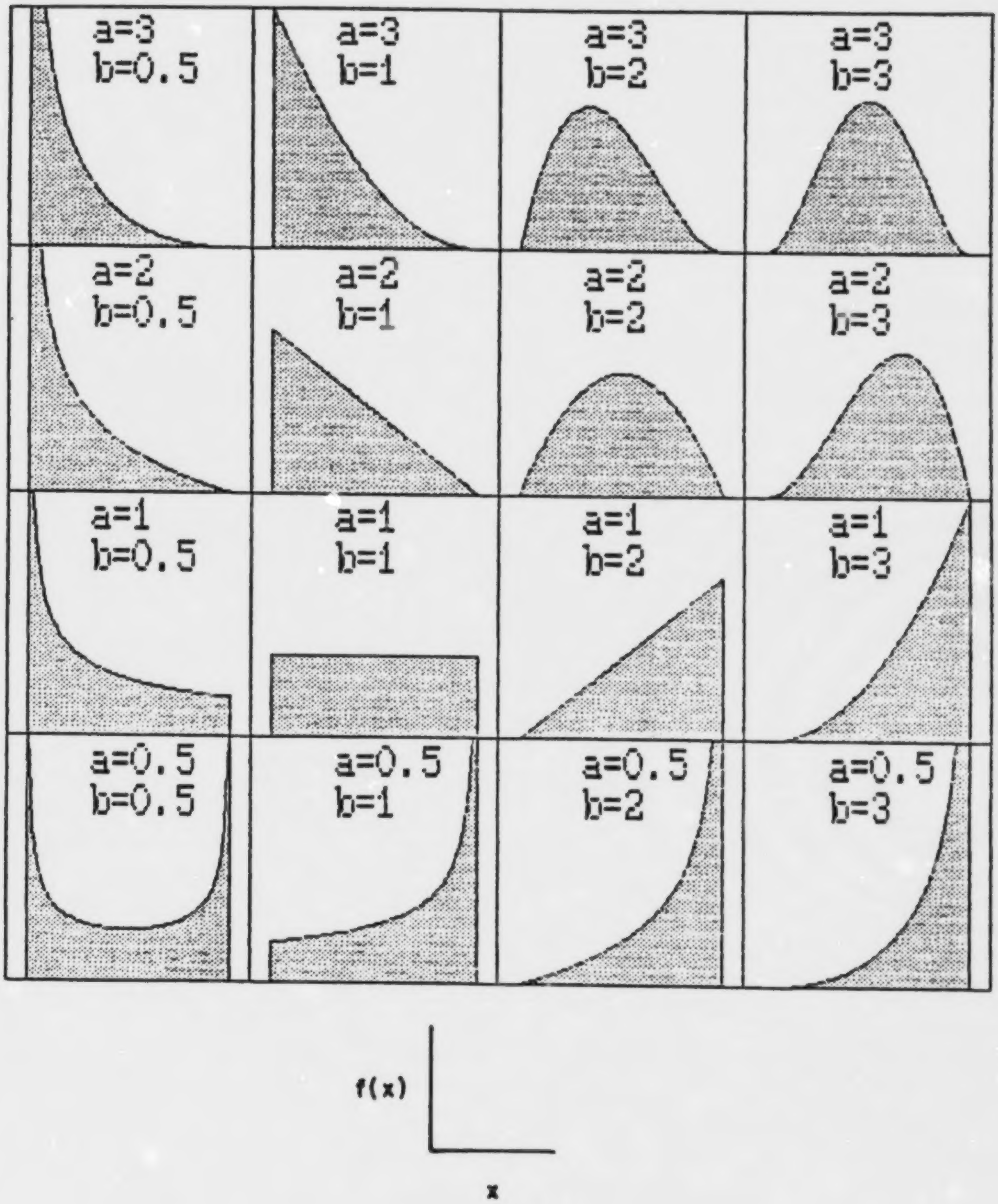
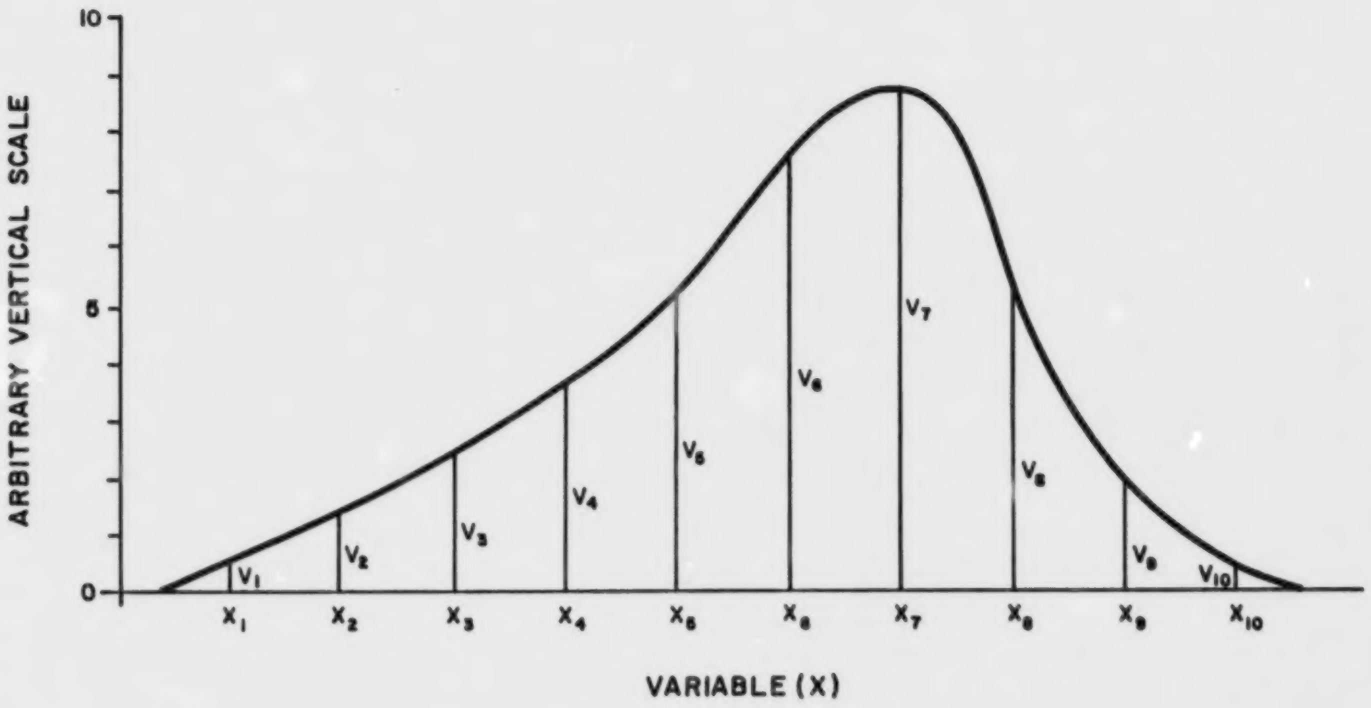


FIGURE 3·4

AN ARBITRARY
PROBABILITY DENSITY FUNCTION



3.1.2 Model Portability

RATAP allows the user to specify input characteristics to meet the criteria of a specific case. Appendix E gives a full listing of the input parameters used and their units. It is important to note that the units for each parameter shown in the listing are maintained throughout the model and changes by the user to the input file should remain consistent with these units.

3.1.3 Deterministic Runs

It is often advantageous, in terms of run time, to run RATAP deterministically rather than running a full probabilistic case. To produce a deterministic run the INPUTD.DAT file is employed. Appendix C lists the INPUTD.DAT file. The difference between INPUTD.DAT and INPUTP.DAT, is that all of the distribution type numbers are set equal to one for constant distributions, and nominal values are specified for each parameter as opposed to specifying distribution descriptors.

3.1.4 Detailed Modular Output

The user has the option to obtain detailed output from any number of modules for one particular month. These output files are different than those specified by the statistics (key file) or the detailed results (res file) files. This option can be accomplished by setting the value corresponding to the appropriate flag, i.e., FLAG1, Table 3.1, to one in INPUTD.DAT. The month for which the data is saved is set with the MONTH flag. By using these two sets of flags it is possible to output key parameters at a particular time of the year.

It should be noted, however, that this option is only recommended with the deterministic run. If used with the probabilistic run the disk space of the computer is quickly exceeded.

3.2 Second Input File (INPUT2.DAT)

The second input file contains the output selection information for the statistics and detailed results output files. Table 3.4 shows a sample file, INPUT2.DAT. The format of this file is described in Table 3.5.

In the first line, the number of months during each year for which an output will be directed to the output files is specified. In the second line, the particular months of interest, e.g. 1 for January and 12 for December, are selected. The count of number of months selected must be in agreement with the count specified in the first line.

The third line of the file specifies the number of arrays to be checked for output. Five variables, BLANK1 through BLANK5, are available to the user for future output of additional parameters. If utilizing one of these variables, changes should be made to the appropriate control modules (see Section 6.4). If more variables are specified then the number being checked for output, those excess variables will be ignored.

The number of outputs from each array in the second input file must be specified. When no output is desired then this number is set to zero. If, however, the number is greater than zero, then the layers from which the output is to be drawn must be specified. This is illustrated on Table 3.5.

3.2.1 Maximum Output Array Size

All of the output going to the detailed results and key files is in the form of an array which has an upper limit of seven hundred fifty elements. To calculate the number of output elements being requested by RATAP you first sum the number of layers output for each of the output variable arrays in the second input file. The number of time variant distributions for which output is desired is then added to this. The resulting number should then be multiplied by the number of months for which output is requested and then multiplied again by the duration of the simulation in years. Finally, added to this number is the number of non-time variant input distributions being

Table 3.4

SAMPLE OF SECOND INPUT FILE (INPUT2.DAT)

```
        Number of months to generate output for each year
 3

        Months to use when generating output (i.e., Jan = 1, Feb = 2,...)
 6   8  10

        Number of arrays to check for output
24
┌────────── Name of array
│    ┌────────── Layers for which to generate output
│    │    ┌────────── Number of layers to be output from array
PH   │    3
     1
     5
     1
PO2       3
RIB       0
R2        0
RPYR      0
PYR       0
FE3       0
AL3       0
FE2       0
CA        0
FE3T      0
SO4T      0
FE2T      0
CAT       0
SO4       0
ALT       0
AFLUX     0
ATOTAL    0
AYEAR     0
BLANK1    0
BLANK2    0
BLANK3    0
BLANK4    0
BLANK5    0
```

Table 3.5

FORMAT OF SECOND INPUT FILE (INPUT2.DAT)

	Column	Format	Description
1 Line:			
	1-3	I3	Number of months each year for which output is desired
2 Line:			
	1-36	12(I3)	Month to use each year for output generation
3 Line:			
	1-3	I3	The number of arrays to check for output
FOR EACH VARIABLE: 1 Line:			
	1-6	A6	Variable name
	7-9	I3	Number of layers to be output from array
FOR EACH LAYER REQUESTED (if any): 1 Line:			
	5-6	I3	Layer number to use to generate output

output. If the final result is more than 750, then the array size limit has been exceeded the program execution will be terminated and an error message will be displayed on the screen.

4.0 COMPILING AND LINKING

Before attempting to run the program each of the following eight modules should be compiled and linked:

INITIAL.FOR
KINETIC.FOR
OXYGEN.FOR
PYRITE.FOR
TRANSPOR.FOR
SPECIATI.FOR
COMEX.FOR
CONTROL.FOR

The file above called CONTROL.FOR is a list of "INCLUDE" statements for the following control module files:

EXEC.FOR
INPUT.FOR
SAMPLE.FOR
SAVE.FOR
STATS.FOR
OUTPUT.FOR

The following files also appear in "INCLUDE" statements in the above files:

IO.INC
STATS.INC
COUNTS.INC
INFO.INC
OUT.INC
INPT.INC
INPT2.INC
UPDATE.INC
PARAM.INC
INTERM.INC
MODEL.INC

All of the above files must be present in order to compile and link the program.

The compiles recommended for RATAP is the $F_{77}L$ compiles by Lahey (1986) version 2.0 on higher. If another compiler is used, problems may ensue.

One potential source of problems in linking is the subroutine "FILER" which calls the $F_{77}L$ and DOS specific functions DATE and TIME and then writes the date and time to the output files. If these functions are not available simply remove this subroutine and the call statements for it in subroutines, INPUT1, WRITE, and OUTPUT (three call statements). Instead, simply write a blank line so that the format of the file is not changed.

The format of the INCLUDE statements used in RATAP is specific to the $F_{77}L$ compiler (Lahey, 1986). While most, if not all, other compilers support INCLUDE statements, their format may not be the same. If errors are encountered while compiling, these statements should be changed to match the syntax of the compiler being used.

To insure the stability of the oxygen module the subroutine UNDERO was used. This subroutine is also specific to the Lahey compiler and will probably not be available on any other compilers. If problems arise while compiling CONTROL.FOR, the call for this subroutine should be deleted from within subroutine INPUT1. The user may, however, experience trouble with the oxygen module due to the multiplication of extremely small numbers.

If the $F_{77}L$ compiler is used, the following options specified in the file "F77L. FIG" are recommended:

```
/a/nf/o/b/i/p/nw/l
```

Further explanation of these options can be found in the user's manual accompanying the compiler.

If the Lahey compiler is used or if a different compiler is used and the option to remember local variables is available, it should not be used.

5.0 RUNNING THE PROGRAM

Before running the program, it should be compiled and linked as described in Section 4.0. The compiler used in developing the program was the Lahey compiler Version 2.2 (1986). Version 2.0 or higher of this compiler is recommended, to facilitate the use of RATAP.

RATAP should be run on a computer having at least 512 kilobytes of Random Access Memory (RAM) and a hard disk drive. A sample session is shown on Table 5.1. The program prompts the user for the names of the input files and indicates, to the screen, the input and output files that are opened.

If errors are encountered in reading these files, messages will be generated accordingly. In some cases, questionable input will result in warning messages, and the user will be asked if it is all right to continue execution of the program or if the program should be stopped. Typing "Y" for yes will cause execution to resume. Either upper or lower case responses are accepted. All error and warning messages are described in Appendix G.

If errors not generated by RATAP occur in reading the input files, check that all real numbers have decimals or are in E format, that no zeroes have been entered as the letter O, and that all counters are correct, particularly for the output selections in the second input file.

While the program is running, the current trial number and time step are written to the screen so that the progress of the program can be checked.

When execution of the program is complete, the output files can be examined. Sample output files are shown in Appendix D.

5.1 Model Test

New RATAP users may wish to run a test on their version of the program. The supplied input files listed in Appendix C have been run successfully with

Table 5.1

SAMPLE SESSION

```
C:UTAP

RATAP

RUN STARTED 02/17/87 AT 13:14:42

First Input File Name? INPUTP.DAT

Opening File : INPUTP.DAT
Opening File : RES.PRB
Opening File : KEY.PRB

Second Input File Name? INPUT2.DAT

Opening File : INPUT2.DAT
Opening File : AVERAGE.DAT



TRIAL NUMBER :     1     TIME :      0
TRIAL NUMBER :     1     TIME :      1
TRIAL NUMBER :     1     TIME :      2
TRIAL NUMBER :     1     TIME :      3
TRIAL NUMBER :     1     TIME :      4
TRIAL NUMBER :     1     TIME :      5

                   ↓

TRIAL NUMBER :    50     TIME :    183
TRIAL NUMBER :    50     TIME :    184
TRIAL NUMBER :    50     TIME :    185
TRIAL NUMBER :    50     TIME :    186


RUN COMPLETED

C:
```

RATAP and the corresponding results are listed in Appendix D. The output values shown for the deterministic run should match exactly with those listed in the Appendix.

6.0 ALTERING THE PROGRAM

As was indicated in the Introduction, the Reactive Acid Tailings Assessment Program is composed of a number of modules. These may be classified as either component or control modules. Component modules (or models) are the programs directly concerned with the simulation of a mine tailings physical system; that is, the mathematical models representing the mine tailings pile. Control modules provide the infrastructure for probabilistic analysis of the component modules. Their functions include probabilistic sampling of input parameters, and many input, output and bookkeeping functions. The integrated control and component modules are referred to as the system model or the Reactive Acid Tailings Assessment Program (RATAP). The general function of the control and component modules are illustrated in Figure 6.1.

The control modules are called in logical order by a primary control module called EXEC. The calling sequence, the interactions between the program EXEC and the other control modules and their functions are illustrated in flowchart form in Figure 6.2. The component module executive subroutine COMEX is called by EXEC for each trial and time step. The subroutine COMEX and the modules it calls are illustrated in Figure 6.3.

The control modules are fully documented in Volume 2 of the report on the Uranium Tailings Assessment Program (SENES, 1986) and updated in the Addendum to Volume 2 (SENES,1987b). Changes made to the control modules by the user should never be required. However, users wishing further detail on the control modules are referred to these sources.

Component module changes should be implemented by following the points outlined below.

6.1 Changing COMEX

Subroutine COMEX is the control module for the component modules. It is called for each time step of each trial. It, in turn, calls the component

FIGURE 6.1

THE SYSTEM MODEL

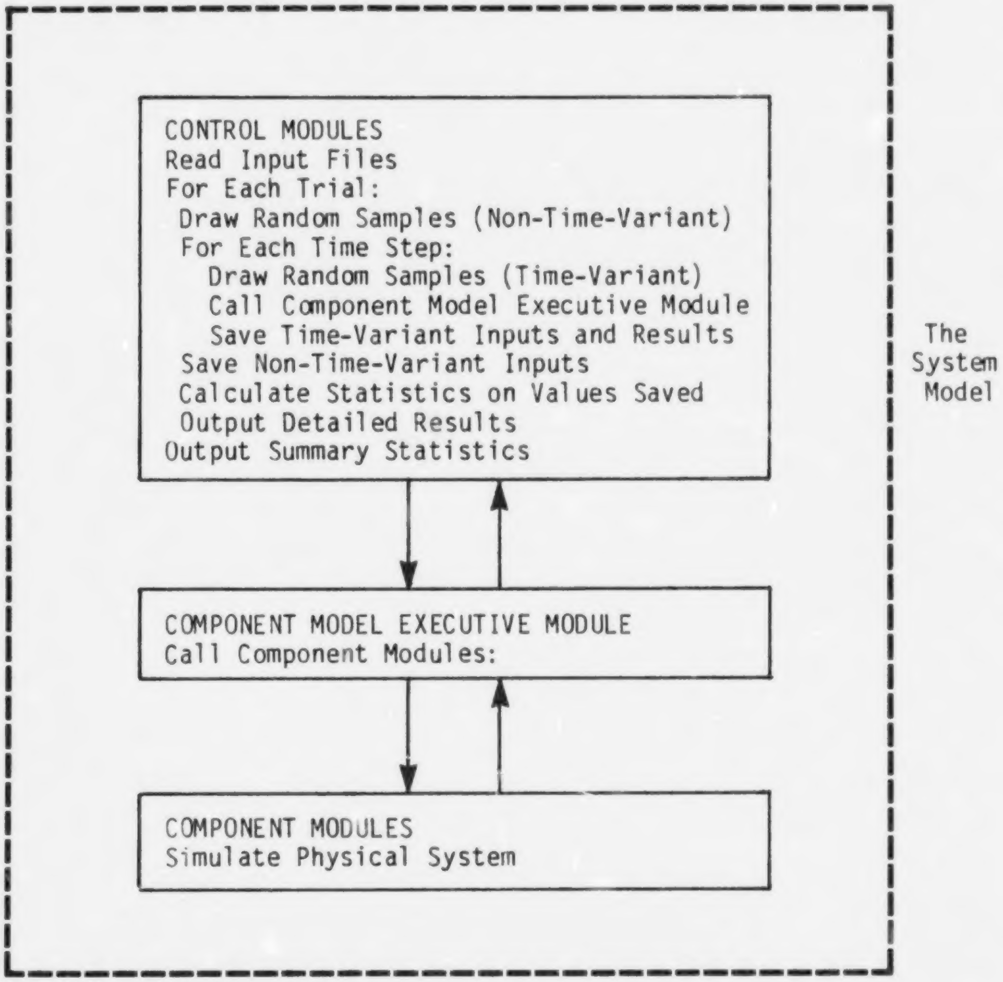

CONTROL MODULES
Read Input Files
For Each Trial:
Draw Random Samples (Non-Time-Variant)
For Each Time Step:
Draw Random Samples (Time-Variant)
Call Component Model Executive Module
Save Time-Variant Inputs and Results
Save Non-Time-Variant Inputs
Calculate Statistics on Values Saved
Output Detailed Results
Output Summary Statistics
COMPONENT MODEL EXECUTIVE MODULE
Call Component Modules:
COMPONENT MODULES
Simulate Physical System
The System Model

FIGURE 6.2
THE CONTROL MODULE STRUCTURE

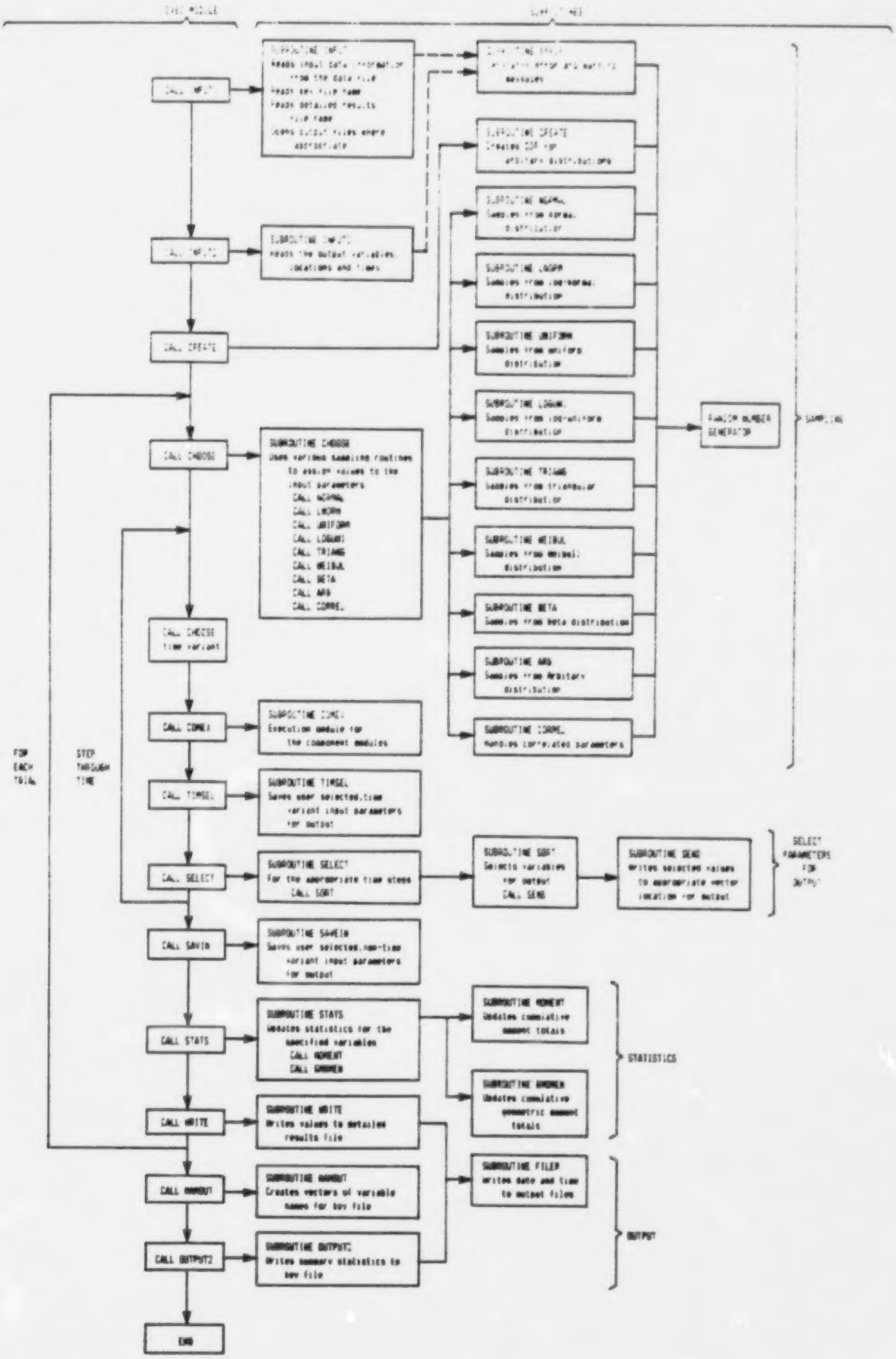
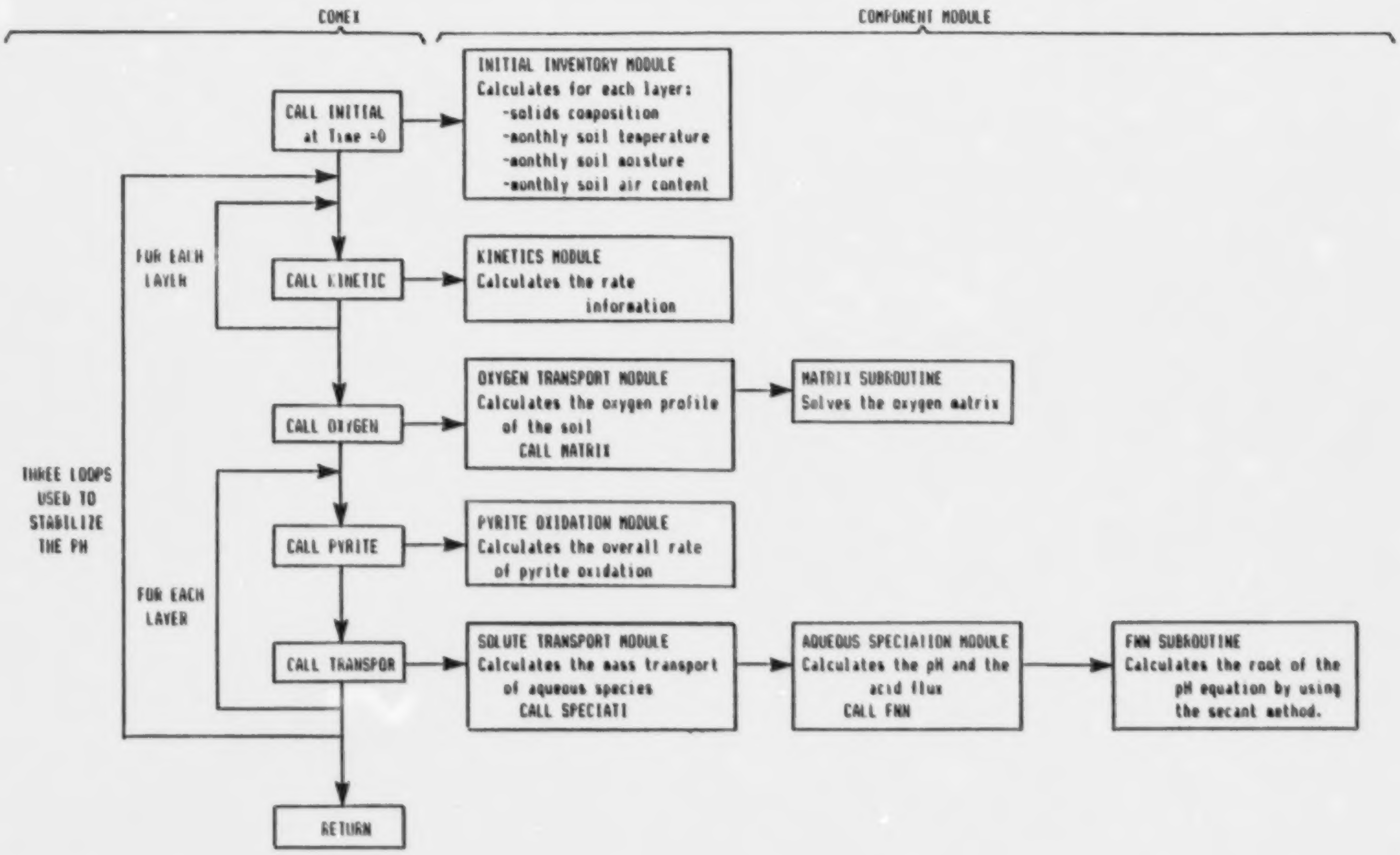

SUBROUTINES
SUBROUTINE INPUT
Reads input data information from the data file
Reads bev file name
Reads detailed results file name
Opens output files where appropriate
SUBROUTINE ERROR
Writes error and warning messages
CALL INPUT
SUBROUTINE CREATE
Creates CDF for arbitrary distributions
SUBROUTINE NORMAL
Samples from normal distribution
CALL INPUT2
SUBROUTINE INPUT2
Reads the output variables, locations and times
SUBROUTINE LNORM
Samples from lognormal distribution
CALL CREATE
SUBROUTINE UNIFORM
Samples from uniform distribution
SUBROUTINE LOGUNI
Samples from log-uniform distribution
RANDOM NUMBER GENERATOR
SAMPLING
CALL CHOOSE
SUBROUTINE CHOOSE
Uses various sampling routines to assign values to the input parameters
CALL NORMAL
CALL LNORM
CALL UNIFORM
CALL LOGUNI
CALL TRIANG
CALL WEIBUL
CALL BETA
CALL ARB
CALL CORREL
SUBROUTINE TRIANG
Samples from triangular distribution
SUBROUTINE WEIBUL
Samples from weibull distribution
SUBROUTINE BETA
Samples from beta distribution
CALL CHOOSE time variant
SUBROUTINE ARB
Samples from Arbitrary distribution
CALL COMEX
SUBROUTINE COMEX
Execution module for the component modules
SUBROUTINE CORREL
Handles correlated parameters
FOR EACH TRIAL
STEP THROUGH TIME
CALL TIMSEL
SUBROUTINE TIMSEL
Saves user selected, time variant input parameters for output
CALL SELECT
SUBROUTINE SELECT
For the appropriate time steps
CALL SORT
SUBROUTINE SORT
Selects variables for output
CALL SEND
SUBROUTINE SEND
Writes selected values to appropriate vector location for output
SELECT PARAMETERS FOR OUTPUT
CALL SAVIN
SUBROUTINE SAVEIN
Saves user selected, non-time variant input parameters for output
CALL STATS
SUBROUTINE STATS
Updates statistics for the specified variables
CALL MOMENT
CALL GMOMEN
SUBROUTINE MOMENT
Updates cumulative moment totals
SUBROUTINE GMOMEN
Updates cumulative geometric moment totals
STATISTICS
CALL WRITE
SUBROUTINE WRITE
Writes values to detailed results file
CALL NAMOUT
SUBROUTINE NAMOUT
Creates vectors of variable names for bev file
SUBROUTINE FILER
Writes date and time to output files
OUTPUT
CALL OUTPUT2
SUBROUTINE OUTPUT2
Writes summary statistics to bev file
END

FIGURE 6.3

THE SUBROUTINE COMEX AND COMPONENT MODULES


COMEX
COMPONENT MODULE
CALL INITIAL at Time =0
INITIAL INVENTORY MODULE
Calculates for each layer:
-solids composition
-monthly soil temperature
-monthly soil moisture
-monthly soil air content
CALL KINETIC
KINETICS MODULE
Calculates the rate information
CALL OXYGEN
OXYGEN TRANSPORT MODULE
Calculates the oxygen profile of the soil
CALL MATRIX
MATRIX SUBROUTINE
Solves the oxygen matrix
CALL PYRITE
PYRITE OXIDATION MODULE
Calculates the overall rate of pyrite oxidation
CALL TRANSPOR
SOLUTE TRANSPORT MODULE
Calculates the mass transport of aqueous species
CALL SPECIATI
AQUEOUS SPECIATION MODULE
Calculates the pH and the acid flux
CALL FNN
FNN SUBROUTINE
Calculates the root of the pH equation by using the secant method.
RETURN
FOR EACH LAYER
FOR EACH LAYER
THREE LOOPS USED TO STABILIZE THE PH

modules. Call statements must be added to COMEX if any new component modules are added.

6.2 Writing Component Modules

All subroutines should be written in Fortran 77 and compiled on the Lahey compiler Version 2.0 or higher (Lahey, 1986) making certain not to use any compiler specific options so as to ensure portability of the program. Variables should be in units corresponding to the rest of the program (see Appendix E).

6.3 Passing Variables

Two files containing input, output, and saved variables are available to the component modeller and should be included in all subroutines.

6.3.1 Include File MODEL.INC

The following common statements and variables contained in the INCLUDE file "MODEL.INC" are necessary for implementing new component modules. This file should be added to component modules, using an include statement. It must not be altered by the user.

a) TIME

This common statement contains the following variables:

T - The current time (Real)
NUMTRL - The trial number
NTRIAL - The total number of trials
NYEARS - Months in simulation (Integer)
NDT - Time increment (Integer)
RYEARS - Years in simulation (Real)
DT - Time increment (Real)

NEWNT - The current time (Integer)
NYR - Number of Years (Integer)

Both integer and real variables are made available to avoid frequent conversion from one to the other throughout the program.

b) INPT

INPT is a common block containing the values sampled from the input distributions. To add new input distributions, the variables should be added to the list in this common block as well as to the first input file. The order of parameters listed in this common block must correspond to the order of the inputs listed in the input files allowed. INPUTP.DAT and INPUTD.DAT. A maximum of 300 inputs is allowed.

6.3.2 Include File INTERM.INC

This file contains a common block to facilitate the transfer of values between subroutines. Included in this file are all of those calculated parameters which appear in more than one module (see Appendix F). Those variables for which output is desired must also be listed in INTERM.INC.

6.4 Obtaining Additional Outputs

The arrays BLANK1, BLANK2, BLANK3, BLANK4, and BLANK5, not used at present, are available for obtaining output for any parameter desired. To do this, the user should go to the end of the subroutine COMEX and equate any positions desired in these arrays to the variable for which output is desired. The position in the array can then be requested for output from the second input file as layer. Note that only variables included in the common block INTERM can be obtained for output in this manner. Additional variables can, however, be added to this common block as described in Section 6.3.2.

As an option to setting BLANK1, BALNK2, BLANK3, BLANK4 and BLANK5 at the end of COMEX, a new subroutine to do this could be called fro the end of COMEX.

6.5 Modifying First Input File

The input files, INPUTP.DAT and INPUTD.DAT should be modified to include all of the input distributions (see Section 3.1) required by the component module. These must be listed in the same order as they appear in the common block INPT. The output files desired should be opened and all counters set to match the number of input distributions.

6.6 Modifying Second Input File

The second input file, INPUT2.DAT, should be modified to obtain the desired output variables, layers, and time steps (see Section 3.2).

REFERENCES

Lahey Computer Systems, Inc., 1986. "$F_{77}L$ - FORTRAN 77 Language System for the Personal Computer." California, U.S.A.

SENES Consultants Limited, 1984. "A Study to Develop and Demonstrate Techniques for the Probabilistic Assessment of the Long-Term Effects of Uranium Mill Tailings in Canada - Phase I." Research Report Prepared for the National Uranium Tailings Program, CANMET, EMR under Supply and Services Canada Contract No. 0SQ83-00236.

SENES Consultants Limited, 1985. "A Study to Develop and Demonstrate Techniques for the Probabilistic Assessment of the Long-Term Effects of Uranium Mill Tailings in Canada - Phase II." Research Report Prepared for the National Uranium Tailings Program, CANMET, EMR under Supply and Services Canada Contract No. 0SQ84-00207.

SENES Consultants Limited, 1986. "Probabilistic Model Development for the Assessment of the Long-Term Effects of Uranium Mill Tailings in Canada - Phase III." Research Report Prepared for the National Uranium Tailings Program, CANMET, EMR under Supply and Services Canada Contract No. 0SQ85-00182.

SENES Consultants Limited and Beak Consultants Limited, 1986. "Estimation of the Limits of Acid Generation by Bacteria-Assisted Oxidation in Uranium Mill Tailings". Research Report Prepared for the National Uranium Tailings Program, CANMET, EMR, under Supply and Services Canada Contract No 0SQ85-00237.

SENES Consultants Limited, 1987a. "Uranium Tailings Assessment Program (UTAP.3): Component Module Documentation". Research Report Prepared for the National Uranium Tailings Program, CANMET, EMR, under Supply and Services Canada Contract No 23317-6-1728/01-SQ

SENES Consultants Limited, 1987b. "Uranium Tailings Assessment Program (UTAP.3): Addendum to Volume 2- System Description and Control Module Documentation ". Research Report Prepared for the National Uranium Tailings Program, CANMET, EMR, under Supply and Services Canada Contract No 23317-6-1728/01-SQ

APPENDIX A

DESCRIPTION OF RATAP

APPENDIX A DESCRIPTION OF RATAP

A.1 Overview of RATAP

The RATAP model is divided into two parts; control modules and component modules. Control modules provide the infrastructure for the probabilistic analysis of the component modules. These modules are responsible for 1) the random selection of values from specified input parameter distributions, 2) performing statistical analysis on user-specified input and calculated parameters and, 3) managing the information transfer between modules. A detailed description of the control modules is presented in Volume 2 of the SENES (1986) report.

Six component modules are employed in the computer code, each performing a specific task. The modules, in order of operation, are: initial inventory, kinetics, oxygen transport, pyrite oxidation, solute transport, and aqueous speciation. The tailings soil profile employed in the component modules is subdivided into distinct zones and a transition zone as indicated on Figure A.1. In the unsaturated zone and capillary fringe, one to twenty layers are employed whereas in the saturated zone, one or two layers are used. The exact number of layers are specified in the input file.

Figure A.2 outlines the call sequence of the modules over time for the various layers. Information transferred between the modules is also identified on the figure. The first module, executed only once, is the initial inventory module which calculates for each layer the initial solids composition, the monthly soil temperature, the soil water content and soil air content. The monthly estimates are assumed to be repeated for each succeeding year.

The kinetics module, the second module, calculates rate information, (the chemical and biological oxidation rates and the oxygen consumption rate) at each time step for the various layers. The calculated parameters transferred into the model are the soil temperatures, water contents, pH and oxygen concentrations; the latter two parameters being estimates. The oxygen

FIGURE A.1
CONCEPT ADOPTED FOR MODELLING OF TAILINGS

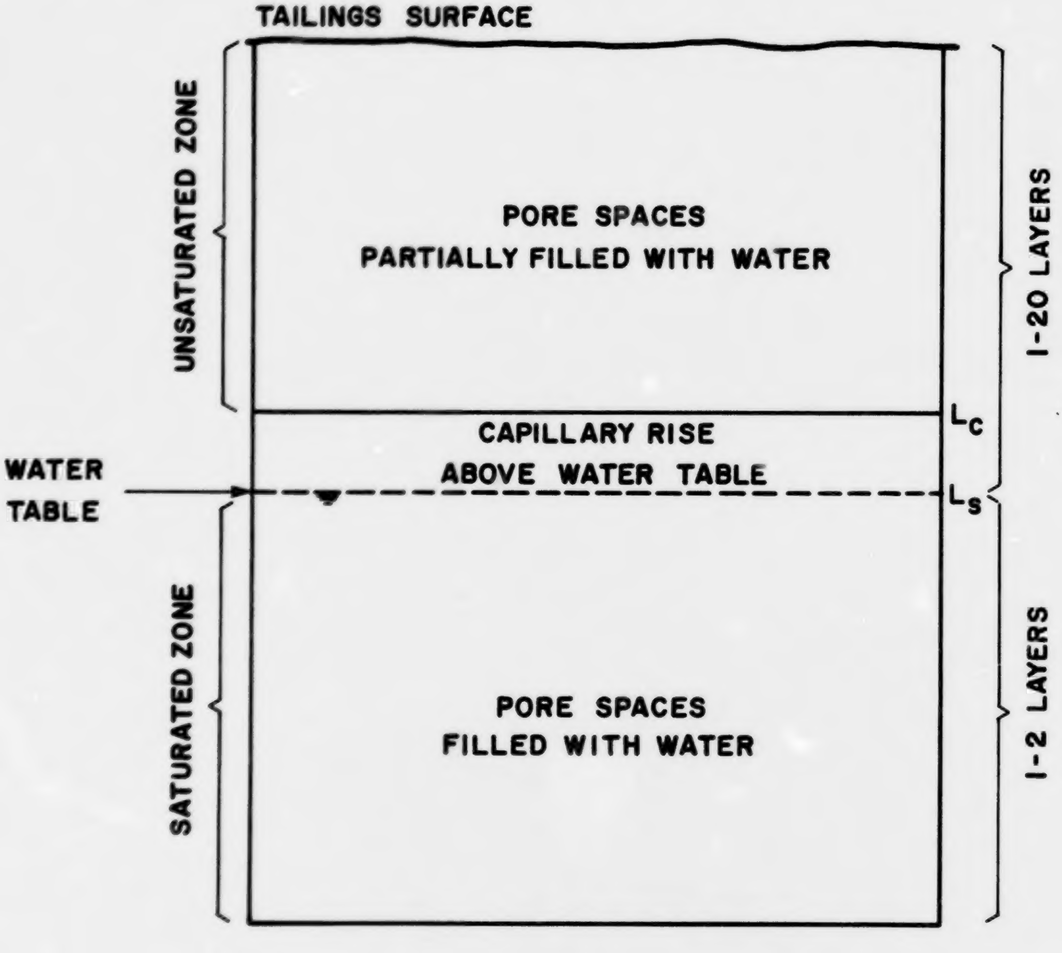
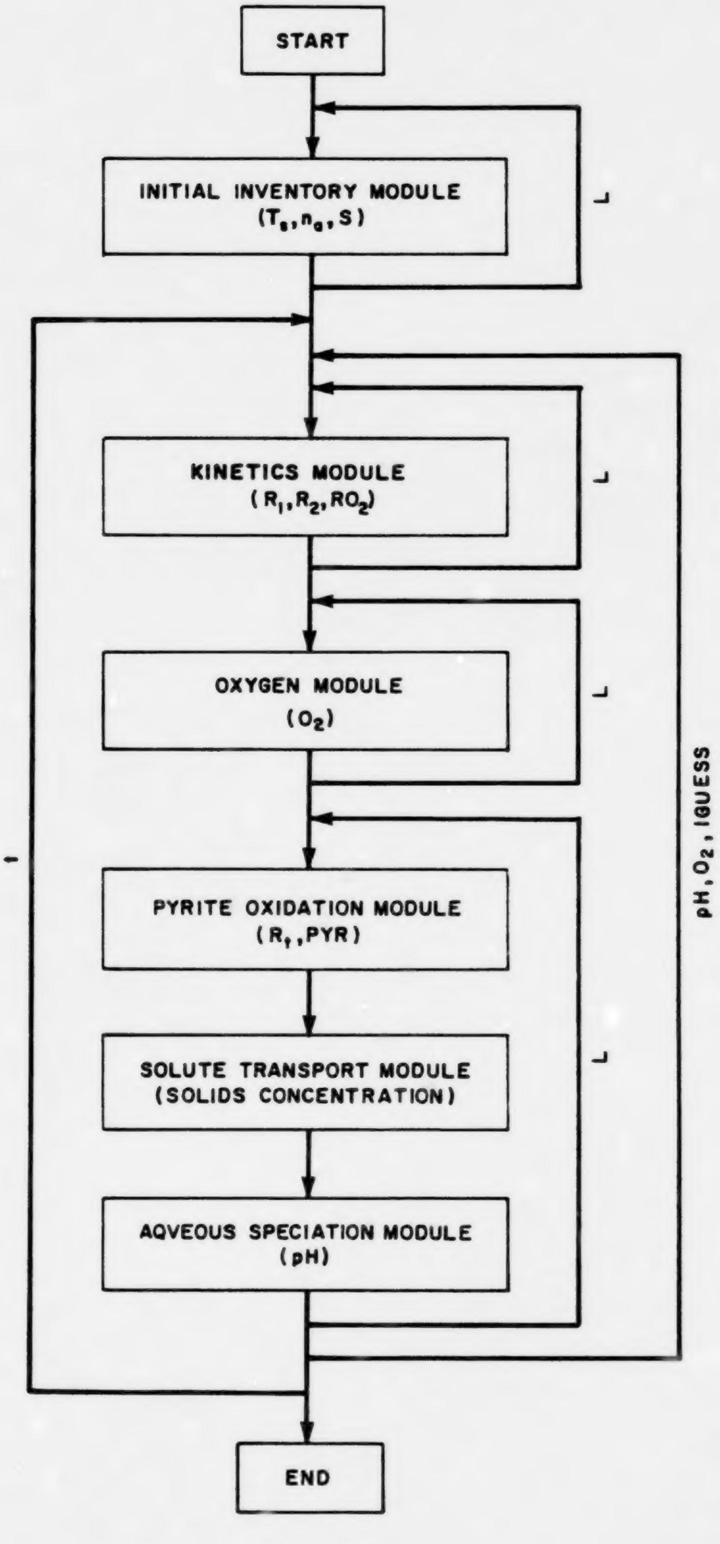

TAILINGS SURFACE
UNSATURATED ZONE
PORE SPACES
PARTIALLY FILLED WITH WATER
1-20 LAYERS
L_C
CAPILLARY RISE
ABOVE WATER TABLE
WATER
TABLE
L_S
SATURATED ZONE
PORE SPACES
FILLED WITH WATER
1-2 LAYERS

FIGURE A.2

CONCEPTUAL FLOW DIAGRAM


START
INITIAL INVENTORY MODULE
(T_s, n_a, S)
KINETICS MODULE
(R_1, R_2, RO_2)
OXYGEN MODULE
(O_2)
PYRITE OXIDATION MODULE
$(R_t$, PYR)
SOLUTE TRANSPORT MODULE
(SOLIDS CONCENTRATION)
AQVEOUS SPECIATION MODULE
(pH)
pH, O_2, IGUESS
END

consumption rate information is then employed in the oxygen transport module, the third module, to calculate the oxygen profile. The oxygen module requires data on the volumetric air content of the soil, in addition to the rate information.

The next three modules (i.e. the pyrite oxidation, solute transport and aqueous speciation modules) are all run in sequence at time t for each layer. The pyrite oxidation module imports the biological and chemical rates of pyrite oxidation and the oxygen concentrations. The pyrite module then adjusts the rates to include the effect of oxygen concentration giving an overall rate of pyrite oxidation. The solute transport and aqueous speciation modules use the rate of pyrite oxidation to calculate the acid flux and pH, respectively. The solute transport and aqueous speciation routines are solved simultaneously.

The pH and oxygen concentrations required for the kinetics module are estimated initially using values from the previous time step. These values are then refined twice by being fed back into the kinetics module and recalculating new values. Test calculations showed that an acceptable convergence of all parameter values was achieved in three iterations. Upon completion of these calculations, the program moves onto time period t+1 and repeats the kinetics through aqueous speciation modules calculations.

The following section briefly outlines the individual modules.

A.2 Initial Inventory Module

In the initial inventory module, initial values for those parameters that are dependent on more than one input are calculated. The parameters can be divided into two broad groups; geochemical parameters and physical parameters.

A.2.1 Geochemical Parameters

The geochemical parameters include an initial estimate of the porewater pH, the aqueous phase concentrations and the solid phase concentrations. The pH estimate is a function of the particular scenario being analyzed, e.g. calcite present or calcite absent.

pH

The porewater pH is estimated by solving the electroneutrality equation. The concentration of other solution ions is estimated from mass balance principles if a solid phase involving the ion is not present, or from chemical equilibrium, if a controlling solid phase is present.

If a particular solid phase is present which buffers pH, the solution pH can be estimated within a narrow range. Hence, the computational procedure can be greatly simplified by employing several pH equations, each applicable for only a particular pH range. Each pH equation is a simplification of the electroneutrality equation; Figure A.3 presents the various solid phase scenarios for which the pH was determined.

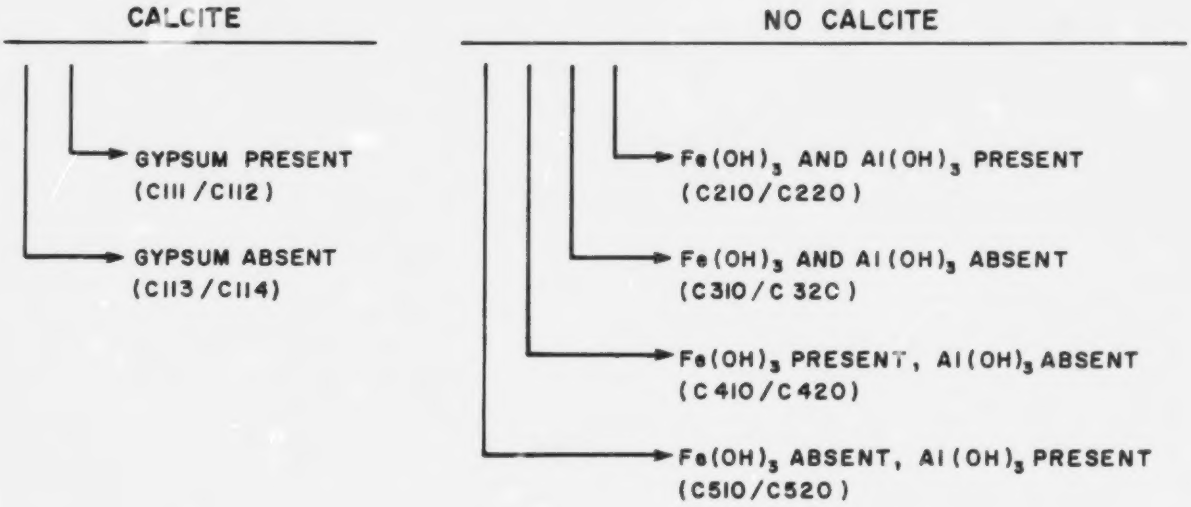
For conditions where calcite is present (i.e. Cases 111 to 114), an exact analytical solution is used to calculate the pH of the tailings porewater. An initial value of 6.5 is assigned, however, to start the program off.

For conditions in which calcite is absent the computational nature of the electroneutrality equation requires that an iterative approach be used to calculate the pH. The secant convergence method is used to solve for the porewater pH. This approach requires two initial estimates of the porewater pH, preferably within 0.5 pH units in order to reduce computational time and instability problems.

For cases where basaluminite is present (i.e. Cases 210/220 and 510/520) initial pH estimates of 4.0 and 3.9 are employed. Similarly the starting pH

FIGURE A.3

pH COMPUTATIONAL SCENARIOS


CALCITE
GYPSUM PRESENT
(C111/C112)
GYPSUM ABSENT
(C113/C114)
NO CALCITE
$Fe(OH)_3$ AND $Al(OH)_3$ PRESENT
(C210/C220)
$Fe(OH)_3$ AND $Al(OH)_3$ ABSENT
(C310/C 32C)
$Fe(OH)_3$ PRESENT, $Al(OH)_3$ ABSENT
(C410/C420)
$Fe(OH)_3$ ABSENT, $Al(OH)_3$ PRESENT
(C510/C520)

NOTE:

C210/C220 DENOTES CASE 210 (UNSATURATED ZONE)
AND CASE 220 (SATURATED ZONE)

for cases in which basaluminite is depleted (i.e. Cases 310/320) and 410/420 is 2.4 and 2.5.

Aqueous Concentrations

In estimating the initial aqueous concentrations of calcium and sulphate, it is assumed that the effect of pyrite oxidation at time zero is minimal. Accordingly, the initial concentration of dissolved calcium and sulfate ions is estimated assuming equilibrium. This gives:

$$[SO_4^{2-}] = [Ca^{2+}] = (K_{CaSO_4}/f_2^{\,2})^{0.5} \qquad (A.1)$$

where
$[SO_4^{2-}]$ = concentration of SO_4^{2-} ($mol.L^{-1}$)
$[Ca^{2+}]$ = concentration of Ca^{2+} ($mol.L^{-1}$)
K_{CaSO_4} = solubility equilibrium constant for $CaSO_4$ ($mol^2.L^{-2}$)
f_2 = activity coefficient for a divalent ion.

The initial solid phase concentrations are calculated using the following equation:

$$C_{si} = \rho_t X_{fi} / M_{wi} \qquad (A.2)$$

where
C_{si} = concentration of component i in the solid phase ($mol.m^{-3}$)
ρ_t = tailings bulk density ($g.m^{-3}$)
X_{fi} = mass fraction of component i in the tailings ($g.g^{-1}$)
M_{wi} = molecular weight of component i ($g.mol^{-1}$)

A.2.2 Physical Parameters

The physical parameters estimated in the initial inventory module are the soil temperature and water content.

Soil Temperature

To estimate soil temperatures the following expression was fitted to experimental data reported by Grenier and Bigu (1983) for the Stanrock tailings management site:

$$T(X,t) = T_m + A_o \, [\sin(w(t-\ell) - X/d)] \;\; \exp(-X/d) \qquad (A.3)$$

where

A_o = empirical coefficient (°K)
w = radial frequency = $2\,\pi/12$ mth (mth^{-1})
d = dampening depth (m)
X = actual depth of layer (m)
T_m = yearly mean temperature (°K)
t = time period (mth)
ℓ = phase-shift constant; a function of the month that represents $t = 1$ (mth)
$T(X,t)$ = soil temperature at depth X at time t (°K)

Water Content

The water content for each layer in the unsaturated zone is determined using the following expression by:

$$n_w = (h_e/h)^{\lambda} \, (n_t - n_r) + n_r \qquad (A.4)$$

where

h_e = an entry value
n_t = the maximum water content, i.e. porosity ($m^3_{void} \cdot m^{-3}_{tail}$)
n_r = the residual water content ($m^3_{water} \cdot m^{-3}_{tail}$)
n_w = the water content of the tailings ($m^3_{water} \cdot m^{-3}_{tail}$)
h = height above water table (m)

λ = soil coefficient; is the material dependent constant that is referred to as the grain size distribution parameter

The form of this equation was developed by Hillel (1980) using experimental measurements for clays and sands. The coefficient values used for sulphidic uranium tailings are based upon best judgement as specific data were not available. It is assumed that for a 10 to 100 year simulation period, the water content profile remains at steady state from month to month.

In the saturated zone the water content is set equal to the porosity:

$$n_w = n_t \qquad (A.5)$$

A.3 Kinetics Module

In the kinetics module the rates of chemical and microbial oxidation of pyritic tailings are calculated. These rates are a function of several environmental parameters.

The oxidation of pyritic tailings is enhanced by the presence of bacteria, principally the group of T. ferroxidans. Bacteria-assisted oxidation of pyrite involves both direct and indirect mechanisms and a sequence of chemical reactions. Direct mechanisms involve attack of the pyrite surface by bacteria while indirect mechanisms include the dissolution of pyrite by ferric ion and the oxidation of ferrous iron resulting from pyrite dissolution by the bacteria. Chemical oxidation involves only the oxidation of pyrite by chemical mechanisms and the subsequent oxidation of the ferrous ion.

A.3.1 Microbial Oxidation

The rate of bacteria-assisted pyrite oxidation, R, is a function, f, of several biological and environmental parameters (Hoffmann et al., 1981; Halbert, et al., 1983; Jaynes et al., 1984; SENES, 1984). It may be stated by the following expression:

$$R = f(X_p, Y_{x/s}, pH, T, P_{O2}, P_{CO2}, S, [N], [P], E_a, A, [I]) \qquad (A.6)$$

where

R = rate of microbial oxidation ($mol.m^{-2}.mth^{-1}$)
X_p = bacterial population density (g biomass per m^2 pyrite surface area)
$Y_{x/s}$ = growth yield coefficient (g biomass per mol pyrite)
pH = measure of hydronium concentration
T = soil temperature (°K)
P_{O2} = oxygen partial pressure (atm)
P_{CO2} = carbon dioxide partial pressure (atm)
S = degree of saturation ($m^3_{water}.m^{-3}_{void}$)
$[N]$ = nitrate or ammonia concentration ($mol.m^{-3}$)
$[P]$ = phosphorus concentration ($mol.m^{-3}$)
E_a = biological energy of activation ($cal.mol^{-1}$)
A = surface area of pyrite (m^2)
$[I]$ = inhibitor concentration ($mol.m^{-3}$)

The overall reaction rate can be expressed as:

$$R_1 = \frac{-\mu X_p}{Y_{x/s}} \tag{A.7}$$

where

R_1 = the specific reaction rate ($mol.m^{-2}_{tailings}.mth^{-1}$)
μ = the specific growth rate (mth^{-1})

A multiplicative expression for the specific growth rate was selected which takes into account temperature, pH, phosphorus concentration, carbon dioxide and moisture content:

$$\mu = \mu_{max}\left[\exp(C_k)\ \underbrace{(\exp(-E_a/R_g\ T))}_{\text{Temperature}}\ \underbrace{(1 + 10^{2.5-pH} + 10^{pH-4.0})^{-1}}_{\text{pH}}\ \underbrace{\left(\frac{[P]}{L_p + [P]}\right)}_{\text{Phosphorus}}\underbrace{\left(\frac{1.3\ P_{CO2}}{10^{-4} + P_{CO2}}\right)}_{\text{Carbon Dioxide}}\ \underbrace{S}_{\text{Moisture}}\right] \tag{A.8}$$

where

μ_{max} = maximum specific growth rate observed (mth^{-1})
L_p = limiting phosphorus concentration ($mol.m^{-3}$)
R_g = universal gas constant ($cal.mol^{-1}.°K^{-1}$)
C_k = constant which sets $\mu = \mu_{max}$ at optimal conditions

The effect of limiting oxygen concentration was not incorporated in the above equation because of the sequence of calculations, i.e. kinetics module first then oxygen module. The effect of oxygen concentration is included in the pyrite oxidation module.

The multiplicative form of the expression is assumed for convenience. It has not, to our knowledge, been unambiguously proven, but is widely used and is assumed to be applicable here.

The constant C_k is set equal to μ_{max} at optimal conditions. It is calculated from the following expression:

$$C_k = \ln \left[(\exp(E_a/R_g\, T_{opt}))\, (1+10^{2.5-pH} + 10^{pH-4.0}) \left(\frac{[P]}{L_p + [P]} \left(\frac{1.3 \quad P_{CO2}}{10^{-4} + P_{CO2}} \right) \quad S \right) \right]^{-1} \qquad (A.9)$$

For the optimal conditions of:

pH = 3.25
T_{opt} = 303°K
E_a = 11700 $cal.mol^{-1}$
R_g = 1.987 $cal.mol^{-1}.°K^{-1}$
[P] = 2.3 $mol.m^{-3}$
L_p = 1.29×10^{-3} $mol.m^{-3}$
P_{CO2} = 3.2×10^{-4} atm
S = 1.0 $m^3_{water} \cdot m^{-3}_{void}$

C_k has a value of 19.737. The value of C_k is only changed when E_a is altered because other "optimum conditions" are invariant. E_a may change due to the inprecision in knowledge of its true (optimum) value.

A.3.2 Chemical Oxidation

The chemical rate of pyrite oxidation in an acid environment is generally much less than the biological oxidation rate at acidic pH values. It is, however, of comparable or greater than the biological rate at neutral to alkaline pH's.

As with the biological rate it is a function of several environmental parameters:

$$R = f\ (pH, T, E_c, A, P_{O2}, S, [Fe^{3+}]) \qquad (A.10)$$

where

$[Fe^{3+}]$ = concentration of the ferric ion ($mol.m^{-3}$)

E_c = chemical energy of activation ($cal.mol^{-1}$)

The specific rate of chemical oxidation has been expressed in the literature (McKay and Halpern, 1958) by the following expression:

$$R_2 = r_c\ P_{O2} \qquad (A.11)$$

where

R_2 = the specific rate of chemical oxidation ($mol.m^{-2}.mth^{-1}$)

r_c = chemical rate coefficient ($mol.m^{-2}.mth^{-1}.atm^{-1}$)

P_{O2} = partial pressure of oxygen (atm)

The chemical rate coefficient is described by:

$$r_c = k_c\ \exp\ (-E_c/R_g\ T) \qquad (A.12)$$

where

T = absolute temperature (°K)

R_g = universal gas constant (1.987 $cal.mol^{-1}.°K^{-1}$)

k_c = chemical rate constant ($mol.m^{-2}.mth^{-1}.atm^{-1}$)

The effect of pH was not included in equation (A.11). Employing experimental data from Smith and Shumate (1970), the following pH expression was developed.

$$f_p = 0.25\ (pH)^{0.70} \tag{A.13}$$

where

f_p = pH factor (dimensionless)

Their data indicated that at a pH of 7.0, $f_p = 1.0$ and at pH of 2.0, f_p = 0.4.

The chemical rate of pyrite oxidation used in this work, then, is:

$$R_2 = f_p\ r_c\ P_{O2} \tag{A.14}$$

Calibration of the expressions using nominal values allowed the relative significance of chemical and biological reactions to be evaluated. At optimal biological conditions (pH=3.25, temperature =30°C, degree of saturation = 1.0, and oxygen concentration = 0.21 atm), the biological reaction rate is 6.5 X 10^{-3} $mol.m^{-2}.mth^{-1}$ while the chemical reaction rate is 7 X 10^{-5} $mol.m^{-2}.mth^{-1}$. These values suggest that the biological rate is about two orders of magnitude greater than the chemical rate at optimal conditions. However, it does not support some literature which suggests that microbially mediated pyrite oxidation can exceed chemical oxidation by a factor of up to 10^6 (Singer and Stumm, 1970).

In tailings optimal biological conditions are seldom attained. Conditions suitable for maximum microbial growth will occur near the tailings surface (i.e. at a degree of saturation of 0.2 and an oxygen partial pressure of 0.21

atm) during the month of July (temperature of 25°C) after calcite has been depleted (pH of 3.6). For these conditions the biological reaction rate is 8.6×10^{-4} mol.m^{-2}.mth^{-1} while the chemical rate is about 5.2×10^{-5} mol.m^{-2}.mth^{-1}. These values suggest that the biological rate is approximately 17 times greater than the chemical rate. This difference is considerably less than that described under optimal conditions.

A.4 Oxygen Module

As indicated in Section A.3 low oxygen concentrations can limit the rate of pyrite oxidation. In the oxygen module the oxygen profile of the tailings is calculated. This information in turn is employed in the calculation of the overall rate of pyrite oxidation.

There are two mechanisms by which oxygen mass transport through a porous medium occurs; advection and diffusion. In the unsaturated zone of soil the diffusive transport of oxygen through the air phase is the dominant transfer mechanism. In the capillary fringe and saturated zones of the tailings the dominant transfer mechanism is advection of oxygen dissolved in the infiltrating porewater. The physical properties of each layer in the gas-filled or non-gas filled tailings zones are used to determine whether gaseous diffusion or advection dominates. The models are described below.

A.4.1 Effective Diffusivity

Diffusive transport is a function of the effective gaseous diffusivity coefficient. The effective gaseous diffusivity (D_e) of the tailings is calculated using the following expression, experimentally determined from Nordic field data (Reardon and Moddle, 1985):

$$D_e = 52.56 \left(\frac{n_a - 0.05}{0.95} \right)^{1.7} \qquad \text{(A.15)}$$

where

n_a = volumetric air content of the soil ($m^3_{air} \cdot m^{-3}_{total}$)
D_e = effective diffusivity of oxygen ($m^2 \cdot mth^{-1}$)

This expression has a lower limit of 0.05 $m^3_{air} \cdot m^{-3}_{total}$ for n_a.

A.4.2 Diffusive Transport

The rate of response of the oxygen profile to changes in gaseous diffusion with time is relatively quick, i.e. in the order of hours compared to slower changes induced by variations in pH and temperature. Accordingly, it is appropriate to assume that the oxygen profile through the gaseous pore spaces of the tailings is at steady state in each monthly time step. This permits the development of analytical solutions for each layer. These equations are coupled to adjoining layers through the appropriate boundary conditions.

There are three possible conditions in each layer which affect the final differential equations and hence their mathematical solution. When pyrite is present, zero-order oxygen consumption kinetics are used at high oxygen concentrations ($P_{O2} > 0.01$ atm) and first order consumption kinetics at low oxygen concentrations. This reflects the fact that oxygen consumption is independent of oxygen concentration at high oxygen concentrations. When pyrite is absent, no consumption of oxygen occurs.

For the first-order consumption reaction at steady state, the analytical solution for flux across any interval where concentrations are known at the boundaries is given as (Carslaw and Jaeger, 1959):

$$F_t = D_e\ (U\ C_1 \cosh\ (U\ dX) - UC_2)/\sinh\ (U\ dX) \qquad (A.16)$$

and

$$F_b = D_e\ (U\ C_1 - U\ C_2 \cosh\ (U\ dX))/\sinh\ (U\ dX) \qquad (A.17)$$

where

F_t = flux at the top of the boundary layer ($mol.m^{-2}.mth^{-1}$)

F_b = flux at the bottom of the boundary layer ($mol.m^{-2}.mth^{-1}$)

C_1 = the oxygen concentration in the upper boundary layer ($mol.m^{-3}$)

C_2 = the oxygen concentration in the lower boundary layer ($mol.m^{-3}$)

U = square root of the ratio of the reaction rate constant (bulk) to the effective diffusivity of the layer $(K_b/D_e)^{0.5}$ (m^{-1})

dX = thickness of a layer (m)

D_e = effective diffusivity through the tailings ($m^2.mth^{-1}$)

K_b = bulk reaction rate constant (mth^{-1})

For a zero-order consumption reaction at steady-state, the fluxes across the layer interfaces are:

$$F_t = R\ dX/2 + D_eC_1/dX - D_eC_2/dX \qquad (A.18)$$

and

$$F_b = -R\ dX/2 + D_eC_1/dX - D_eC_2/dX \qquad (A.19)$$

where

R = zero-order rate constant ($mol.m^{-3}.mth^{-1}$)

When pyrite (the sulfide mineral) is not present, the diffusive flux is simply expressed by Fick's first law:

$$F = D\ (C_1 - C_2)\ /dX \qquad (A.20)$$

where

F = the flux of oxygen across the top boundary ($mol.m^{-2}.mth^{-1}$)

The effective diffusivity coefficient, D_e, is estimated from equation (A.15). The zero-order reaction rate constant is estimated from the biological and chemical reaction rate constants as:

$$R = 3.75\ (R_1 + R_2)\ \frac{\alpha_p}{V_g} \qquad (A.21)$$

where

R = zero-order reaction rate constant ($mol.m^{-3}.mth^{-1}$)
R_1 = biological reaction rate constant ($mol.m^{-2}.mth^{-1}$)
R_2 = chemical reaction rate constant ($mol.m^{-2}.mth^{-1}$)
α_p = pyrite surface area per unit volume tailings ($m^2.m^{-3}$)
V_g = volume of gas per unit volume of tailings ($m^3.m^{-3}$)

The factor, 3.75, is a stoichiometic factor (mole O_2 consumed per mole pyrite oxidized).

A.4.3 Advection Transport

In water saturated soil the gaseous diffusivity is small. The major transport route for oxygen is via infiltrating water. This advective flux however, is small relative to transport by gaseous diffusion in the unsaturated zone. It provides a boundary condition at the water table and can be expressed as:

$$F = V\ C_w\ K_H \qquad (A.22)$$

where

C_w = the concentration of oxygen (in solution) at the air-water boundary ($mol.m^{-3}$)
V = the rate of infiltration of water ($m.mth^{-1}$)
K_H = Henry's Law Constant ($m^3.m^{-3}$)

A.4.4 Overall Mathematical Solution

Oxygen transport and oxygen consumption are described by coupling the various solutions at the appropriate boundaries. Different combinations of consumption in adjoining layers give different analytical solutions for each interface dependent upon the conditions involved. This results in 6 possible equations that can apply to the top boundary, 6 equations for intermediate boundaries and 3 equations for the bottom boundary.

The general equation that applies to all conditions has a linear algebraic form which in matrix notation, is:

$$\underline{A}\ \underline{C} = \underline{W} \qquad (A.23)$$

where

$\underline{A}$ = the matrix of coefficients ($m.mth^{-1}$)
$\underline{C}$ = the concentration of oxygen with depth ($mol.m^{-3}$)
$\underline{W}$ = the loading term ($mol.m^{-2}.mth^{-1}$)

$\underline{A}$ is an nxn matrix, and $\underline{C}$ and $\underline{W}$ are nx1 matrices. There are up to 3 coefficients in each row of $\underline{A}$ having a non zero value. The values of these coefficients change due to the 15 different conditions possible. The $\underline{A}$ matrix is tridiagonal with the dominant diagonal containing the A coefficients for the middle interface and the upper and lower diagonals containing the upper and lower interface coefficients respectively. The mathematical solution for C is found by simultaneous solution of the N equations where N equals the number of interfaces or layers.

A.5 Pyrite Oxidation Module

In the pyrite oxidation module the depletion of the pyrite content in the tailings is calculated. The effects of oxygen concentration, pyrite surface area and the kinetic rate constants are employed in the calculation of the overall reaction rate.

The overall reaction rate for pyrite oxidation can be expressed as:

$$\frac{dM}{dt} = \frac{-A_p}{V} (R_{1b} + R_2) \qquad (A.24)$$

where

M = moles of pyrite per unit volume of tailings ($mol.m^{-3}$)
R_{1b} = biological specific reaction rate per unit area of pyrite ($mol.m^{-2}mth^{-1}$)
R_2 = chemical specific reaction rate per unit area of pyrite ($mol.m^{-2}.mth^{-1}$)
A_p = surface area of pyrite (m^2)
V = volume of tailings (m^3)
t = time (mth)

A.T.1 Rate Limitation due to Oxygen Concentration

The biological reaction rate constant defined above, R_{1b}, is effectively a "material" constant and is independent of oxygen concentration. The net biological oxidation rate is equal to this "material" constant times an oxygen factor. The limiting effect of oxygen on the biological specific reaction rate can be included in equation (A.24) by replacing the term R_{1b} with:

$$R_{1b} = R_1 \frac{P_{O_2}}{L_o + P_{O_2}} \qquad (A.25)$$

where

P_{02} = partial pressure of oxygen (atm)
L_o = limiting oxygen partial pressure (atm)
R_{1b} = oxygen influenced biological specific reaction rate ($mol.m^{-2}.mth^{-1}$)

This equation includes the influences of oxygen concentration using a Monod type expression. It is essentially equivalent to the zero order and first order rate expressions used in the oxygen model: it has a value equivalent to the zero order constant (R_1) at high oxygen concentrations and equivalent to the first order rate constant $k_b = R_1/L_o$ at low oxygen concentrations where $L_o = .01$.

The chemical term, R_2 in equation (A.24), incorporates a first order oxygen dependence:

$$R_2 = f_p \; k_c \; P_{O2} \qquad \text{(A.26)}$$

where:

k_c = chemical rate constant ($mol.m^{-2}.mth^{-1}.atm^{-1}$)
R_2 = chemical specific reaction rate ($mol.m^{-2}.mth^{-1}$)
f_p = pH dependence factor

Oxygen dependence of pyrite oxidation upon the chemical and biological kinetics results in a mixed dependence which is neither Monod nor first order. As indicated above, the biological component is much larger than the chemical component over much of the acidic pH range, the range of concern for this project. This allowed the simplifying assumption that the overall oxygen dependence is essentially a Monod expression. Subsequent inspection of this assumption involving analysis of calculated fluxes, showed that this assumption was justified.

A.5.2 Effect of Particle Size Distribution

As oxidation proceeds the surface area of individual pyrite particles decreases. The rate at which the pyrite particle "shrinks" due to dissolution by oxidation is given by the following expression:

$$\frac{dM}{dt} = +\left(\rho_p \frac{A_p}{V}\right) \frac{dr}{dt} \qquad \text{(A.27)}$$

where:

ρ_p = moles of pyrite per volume of pyrite ($mol.m^{-3}$)
r = average radius of pyrite particles (m)

V = volume of tailings (m^3)
A_p = total surface area of pyrite particles (m^2)

The expression assumes that the pyrite particles are spherical.
The overall rate of pyrite oxidation can be determined by combining equations (A.24) and (A.27):

$$-\left(\frac{\rho_p}{V} \quad A_p\right)\frac{dr}{dt} = \frac{A_p}{V} \quad (R_{1b} + R_2) \qquad \text{(A.28)}$$

or

$$-\frac{dr}{dt} = \frac{R_t}{\rho_p} \qquad \text{(A.29)}$$

where

R_t = overall specific reaction rate, (i.e. $R_{1b} + R_2$) ($mol.m^{-2}.mth^{-1}$)

Integration of equation (A.29) by assuming that R_t is constant for the time period "0 to t" yields:

$$r = r_o - \left(\frac{t \ R_t}{\rho_p}\right) \qquad \text{(A.30)}$$

which can be expressed alternatively as:

$$r = r_o - k_o \ t \qquad \text{(A.31)}$$

where
r_o = initial radius of particle (m)
k_o = rate constant for oxidation ($m.mth^{-1}$)

Substitution of a term for the concentration of pyrite remaining, moles of pyrite per m^3 of tailings, as a function of surface area and time gives:

$$M_{r,t} = M_{r,0}\left(\frac{r - k_o \ t}{r_o}\right)^3 \qquad \text{(A.32)}$$

for $r \geq k_o \ t$.

The initial radii of pyrite grains in tailings however, are not of a uniform size, but have various sizes. The radii can be described by the following size distribution density function:

$$f(r) = \frac{x\,\alpha}{r_m}\left(\frac{r}{r_m}\right)^{\alpha-1} + \frac{y\,\beta}{r_m}\left(\frac{r}{r_m}\right)^{\beta-1} \qquad (A.33)$$

where

$f(r)$ = size distribution density function
r_m = maximum radius of particles (m)
x, y, α, β = Paretto distribution function coefficients ($x + y = 1$)

By substituting equation (A.33) into equation (A.32) and integrating results in the following polynomial expression:

$$M_t = M_o\left[1 + a_1\left(\frac{k_o\,t}{r_m}\right)^{\alpha} + a_2\left(\frac{k_o\,t}{r_m}\right)^{\beta} + a_3\left(\frac{k_o\,t}{r_m}\right) + a_4\left(\frac{k_o\,t}{r_m}\right)^{2} + a_5\left(\frac{k_o\,t}{r_m}\right)^{3}\right] \qquad (A.34)$$

where:

M_o = initial pyrite concentration in moles per unit volume of tailings ($mol.m^{-3}$).

r_m = the initial maximum radius and $k_o\,t \leq r_m$

$$a_1 = -x\left(1 - \frac{3\alpha}{\alpha-1} + \frac{3\alpha}{\alpha-2} - \frac{\alpha}{\alpha-3}\right)$$

$$a_2 = y\left(1 - \frac{3\beta}{\beta-1} + \frac{3\beta}{\beta-2} - \frac{\beta}{\beta-3}\right)$$

$$a_3 = -\left(\frac{3x\alpha}{\alpha-1} - \frac{3y\beta}{\beta-1}\right)$$

$$a_4 = \frac{3x\alpha}{\alpha-2} - \frac{3y\beta}{\beta-2}$$

$$a_5 = -\left(\frac{x\alpha}{\alpha-3} - \frac{y\beta}{\beta-3}\right)$$

Once the pyrite concentration has been determined, the relationship between surface area and volume of tailings can be calculated for any time by differentiating equation (A.34) to give:

$$\alpha_p = \frac{-M_o}{\rho_p\, r_m}\left[a_1\, \alpha\left(\frac{k_o\, t}{r_m}\right)^{\alpha-1} + a_2\, \beta\left(\frac{k_o\, t}{r_m}\right)^{\beta-1} + a_3 + 2a_4\left(\frac{k_o\, t}{r_m}\right) + 3a_5\left(\frac{k_o\, t}{r_m}\right)^2\right] \qquad (A.35)$$

A.6 Solute Transport Module

In the solute transport module, the mass transport of aqueous species via percolating water, and a solids balance are determined. The particular algorithms employed in the calculations are a function of the presence or absence of various minerals such as calcite, gypsum and solids containing aluminum and iron.

The solute transport model assumes that water infiltrates vertically down through the unsaturated zone to the saturated zone in a plug flow manner. From the saturated zone, water flows horizontally to surface water and vertically downward to deep subsurface flow (i.e. groundwater). Transport calculations depend on two types of dissolution machanisms: kinetically-controlled dissolution, and equilibrium controlled dissolution. Evidence available from the literature justifies the assumption that the dissolution of sericite and pyrite is kinetically controlled and that the dissolution of calcite, gypsum, basaluminite, and goethite is equilibrium controlled for the monthly-time-scales of interest here (Beak, 1985).

For elements like potassium leached from sericite, the mass balance equation gives:

$$\left[K_i\right] = \frac{q_{i-1}\,[K_{i-1}] + f_K \cdot r_{ser} \cdot V_i}{q_i} \qquad \text{(A.36)}$$

where

$[K_i]$, $[K_{i-1}]$ = the potassium concentration in water leaving layer i and layer i-1 respectively ($mol^{-1}.L$)
q_i, q_{i-1} = the flow rate leaving layer i and layer i-1 respectively ($L.mth^{-1}$)
r_{ser} = the sericite dissolution rate (mol sericite.m^{-3} tailings.mth^{-1})
f_K = the stoichiometry factor (mol potassium released. mol^{-1} sericite dissolved)
V_i = the volume of layer i (m^3)

The term $f_K.r_{ser}.V_i$ is the source of potassium from sericite dissolution ($mol.mth^{-1}$).

A mass balance on sericite gives the following equation for the solid phase:

$$[Ser_t] = [Ser_{t-1}] - r_{ser}\, dt \qquad \text{(A.37)}$$

where

$[Ser_t]$ = the mass inventory of sericite at time t ($mol.m^{-3}$)
dt = the elapsed time between t-1 and t (mth)

These two equations are applicable for kinetically controlled dissolution. Equation (A.36) is applicable for aluminum provided that no other solid phase exists by substituting $[Al_T]$ for [K] and the stoichiometric factor (mole Al released per mole sericite dissolved). Here $[Al_T]$ is the total aqueous concentration of Al, including solution complexes. Where basaluminite exists or thermodynamic formation is predicted, then equilibrium conditions control the aqueous ionic concentration of aluminum $[Al_i]$. Basaluminite ($Al_4(SO_4)(OH)_{10}$) was used here to describe solubility controls for Al. This choice was based on the findings of Dubrovsky et al. (1985) for the Nordic tailings which suggested that this solid phase better describes the observed solution concentrations than does the $Al(OH)_3$ solid phase. In this case:

$$[Al_i] = \frac{1}{f_3}\left(\frac{10^{KBAS - 10pH}}{f_2\,[SO_4^{2-}]}\right)^{0.25} \qquad (A.38)$$

where

f_2, f_3 = activity coefficients for 2^+ and 3^+ sericite species
$[SO_4^{2-}]$ = the solution sulfate concentration ($mol.L^{-1}$)
KBAS = the power for the basaluminite solubility constant.

Because the ionic concentration of aluminum is a function of pH and sulfate concentration, its value is simultaneously obtained with the solution of the equation for pH (see below).

For an element such as aluminum which dissolves and which may participate in formation of another solid, the solid's mass balance is:

$$[BAS]_t = [BAS]_{t-1} + (q_{i-1}\,[Al_T]_{i-1} + f_{Al}\, r_{ser}\, V_i - q_i\,[Al_T]_i)\, dt \qquad (A.39)$$

where

$[BAS]_t$ = the basaluminite concentration ($mol.m^{-3}$)

f_{Al} = the aluminum sericite stoichiometry factor

$[Al_T]_{i-1}$ = the total aqueous aluminum concentration in layer i-1 ($mol.\ m^{-3}$)

For other elements such as Fe^{3+}, Ca^{2+}, SO_4^{2-}; similar equations are used to solve for the aqueous concentrations and inventories, dependent upon whether or not a solid phase exists at equilibrium with solution. The only changes involved are formulation of the equilibrium relationship analogous to equation (A.40) (Fe^{3+} with goethite; Ca^{2+} with gypsum and calcite; and SO_4^{2-}-with gypsum) and of the presence or absence of a kinetic term in equation (A.39) (pyrite is the only other solid with a kinetic term).

The mass balance for Fe^{3+} and Fe^{2+} has an added complicating factor: in a net sense a portion of the pyrite oxidized forms Fe^{3+} while the remainder forms Fe^{2+}. This occurs because Fe^{3+} is formed by bacterial oxidation but is reduced to Fe^{2+} during the dissolution of pyrite. This results in a source for Fe^{3+}:

$$Source_{Fe3} = (0.02 + P_{02}{}^{1/2}).R_{pyr}.\ V_i \qquad (A.40)$$

and the source for Fe^{2+}:

$$Source_{\ Fe2} = \left(\frac{0.46 - P_{02}{}^{1/2}}{0.48}\right).R_{pyr}.V_i \qquad (A.41)$$

These are empirical relationships based on laboratory data.

Under reducing conditions ($P_{02} = 0$), pyrite can be dissolved by Fe^{3+} entering a tailings layer with infiltrating rainwater. The net overall reaction results in an additional source term for Fe^{2+} and a sink term for Fe^{3+} under reducing conditions. The equations are:

$$\mathrm{Source}_{Fe2} = -\mathrm{Sink}_{Fe3}$$

$$= -K_{Fe3}\,[Fe^{3+}T]\,\frac{L_{O2}}{L_{O2} + P_{O2}}\ \exp\left[\frac{-E_{a2}}{1.987}\left(\frac{1}{T} - \frac{1}{298}\right)\right] V_i \qquad (A.44)$$

where

K_{Fe3} = the reaction rate constant (mth^{-1})
E_{a2} = the activation energy of the reaction ($cal.mol^{-1}$)
T = the ground temperature (°K).

A.7 Speciation Module

The main purpose of the speciation module is the calculation of the pH and the acid flux. The calculation of pH is based upon the principle of electroneutrality. For the ions of concern in this equation, it is:

$$10^{-pH} + 2[Ca^{2+}] + ALUM + IRON + 2[Fe^{2+}] + [K^+] = [HCO_3^-] + SULF + [NO_3^-] \qquad (A.45)$$

where

$$\begin{aligned} ALUM = {} & (3 + 2\,f_3\,CAlOH\,10^{pH}/f_2 + f_3\,CAlOH_2\,10^{2pH}/f_1 + \\ & + f_3\,CAlOH_3\,10^{3pH} + f_3\,f_2\,CAlSO4\,[SO_4^{2-}]/f_1)\,[Al^{3+}] \end{aligned} \qquad (A.46)$$

$$\begin{aligned} IRON = {} & (3 + 2\,f_3\,CFeOH\,10^{pH}/f_2 + f_3\,CFeOH_2\,10^{2pH}/f_1 + \\ & + f_3\,CFeOH_3\,10^{3pH} + f_3\,f_2\,CFeSO_4\,[SO_4^{2-}]/f_1)\,[Fe^{3+}] \end{aligned} \qquad (A.47)$$

$$SULF = (2 + f_2\,10^{-pH}/(CHSO_4\,f_1))[SO_4^{2-}] \qquad (A.48)$$

where

$CAlOH$, $CAlOH_2$, $CAlOH_3$, $CAlSO_4$,

$CFeOH$, $CFeOH_2$, $CFeOH_3$, $CFeSO_4$ = thermodynamic complexation constants

f_1, f_2 and f_3 = activity coefficients

All chemical concentrations refer to layer i whether or not explicitly 'subscripted with "i". The term 'ALUM', 'IRON', and 'SULF' refer to solution complexes of aluminum, iron and sulfate which have a charge. For 'ALUM' and 'IRON', the respective complexes in equation (A.46) and (A.47) are the 3+, (Al^{3+}, Fe^{3+}), 2+ ($AlOH^{2+}$, $FeOH^{2+}$), the 1+ ($Al(OH)_2^+$, $Fe(OH)_2^+$) and sulfate, $AlSO_4^+$, $FeSO_4^+$) complexes. For sulfate, equation (A.48), the respective species are SO_4^{2-} and HSO_4^-.

The $[Al^{3+}]$ is estimated from the solubility constant and pH if the solid phase is present, but from $[Al_T]$ (from solution mass balance) and pH if no solid phase is present. $[Fe^{3+}]$ is estimated similarly. $[Ca^{2+}]$ and $[SO_4^{2-}]$ are estimated from equilibrium considerations if gypsum is present and from solution mass balance if it is absent. If calcite is present, $[Ca^{2+}]$ is estimated from gypsum equilibria and $[HCO_3^-]$ is estimated from the following expression for tailings layers which are not fully saturated:

$$[HCO_3^-] = \frac{K_H \, K_1 P_{CO2}}{f_1 \, 10^{-pH}} \qquad (A.49)$$

K_1 = the dissociation constant for carbonic acid ($mol.L^{-1}$)
K_H = solubility constant for carbon dioxide ($mol.L^{-1}.atm^{-1}$)
P_{CO_2} = the partial pressure of carbon dioxide (atm)
$[HCO_3^-]$ = the bicarbonate concentration ($mol.L^{-1}$)

For saturated tailings layers,

$$[HCO_3^-] = \frac{K_1}{f_1 \, 10^{-pH} + K_1} C_T \qquad (A.50)$$

where

C_T = the total inorganic carbon concentration in solution, calculated by mass balance (mol.L^{-1})

The pH is calculated by finding the root of equation (A.45) (i.e. where the L.H.S. equals the R.H.S.) using an iterative search technique.

The two routines, transport and speciation are solved simultaneously depending upon which solid phases are present. Generally solution mass balance calculations are first made, the pH estimated, and then the remaining mass balance calculations are made (for solid phases, and solution phases if a solid phase completely dissolves during a time step).

A.8 References

Beak Consultants, 1985. "Descriptive Algorithm Development for Physical, Chemical and Biological Processes Operational in Uranium Mill Tailings", Research report prepared for the National Uranium Tailings Program, CAMET, EMR.

Carslaw, H.S. and Jaeger, J.C., 1959. Conduction of Heat in Solids, Oxford University Press, Oxford, Great Britain.

Dubrovsky, M.M., Cherry, J.A., Reardon, E.J., and Vivyurka, A.J., 1985. "Geochemical Evolution in the Elliot Lake Uranium District", Canada Geo. Tech. Journal, Vol 22, pp. 110-128.

Grenier, M.G., and Bigu, J., 1983. "Analysis of Seasonal Variations in Soil Temperature at a Uranium Tailings Disposal Site - A Comparison with Theoretical Data." CANMET, Minerals Research Program, Elliot Lake Laboratory, Division Report MRP/MRL 83-84.

Halbert, B.E., Scharer, J.M., Knapp, J.A., and Gorber, D.M., 1983. "Determiniation of Acid Generation Rates in Pyritic Mine Tailings." presented at the 56th Annual Conference of the Water Pollution Control Federation, October 2-7, Atlanta, Georgia.

Hillel, D., 1980. Fundamentals of Soil Physics, Academic Press, New York, N.Y.

Hoffmann, M.R., Faust, B.C., Panda, F.A., Koo, H.H., and Tsuchiya, H.M., 1981. "Kinetics of the Removal of Iron Pyrite from Coal by Microbial Catalysis." Appl. and Env'tl. Microbiol., Vol. 42, pp. 259-271.

Jaynes, D.B., Rogouski, A.S., and Pionke, H.B., 1984. "Acid Mine Drainage from Reclaimed Coal Strip Mines; 1. Model Description." Water Resources Research, Vol. 20, No. 2, pp. 233-242, February.

McKay, D.R., Halpern, J., 1958. "A Kinetic Study of the Oxidation of Pyrite in Aqueous Suspension." Trans. Metall. Soc. AIME 212, pp. 301-309.

Reardon, E.J., Moddle, P.M., 1985. "Gas Diffusion Coefficient Measurements in Uranium Mill Tailings: Implications to Cover Layer Design". Preprint to Reclamation and Revegetation Research.

SENES Consultants Limited, 1984. "Report on the Assessment of the Mechansism of Bacterially-Assisted Oxidation of Pyritic Uranium Tailings." Research Report Prepared for the National Uranium Tailings Program, CANMET, EMR, Ottawa.

SENES Consultants Limited, 1986. "Probabilistic Assessment of Uranium Mill Tailings: Phase III". Research Report Prepared for the National Uranium Tailings Assessment Program, CANMET, EMR, Ottawa.

Singer, P.C., and Stumm, W., 1970. Science, Washington, D.C., No. 167, pp. 1121.

Smith, E.E., and Shumate, K.S., 1970. Water Poll. Cont. Res., Report No. 14010 FPS DAST-40, U.S. Dept. Int., FWPCA.

APPENDIX B

COMPUTER CODE

APPENDIX B COMPUTER CODE

B.1 MODULES

The computer codes for RATAP's control and component modules are presented on the following pages in alphabetical order.

The followings is a list of the modules:

Component Modules

- COMEX.FOR
- CONTROL.FOR
- INITIAL.FOR
- KINETIC.FOR
- PYRITE.FOR
- SPECIATI.FOR
- TRANSPOR.FOR

Control Modules

- EXEC.FOR
- INPUT.FOR
- OUTPUT.FOR
- SAMPLE.FOR
- SAVE.FOR
- STATS.FOR

```
C FILE 'COMEX.FOR'

      SUBROUTINE COMEX

C     CONTROL MODULE FOR COMPONENT MODULES

      INCLUDE 'MODEL.INC'
      INCLUDE 'INTERM.INC'
C
C
      IF ( T .EQ. 0.) THEN
         XFLAG = 0.
      ENDIF
C
      IF (XFLAG .NE. 1.) THEN
C
C       READ DUMMY SOURCE FILES
C
C       DETERMINING THE PARTICULAR MONTH
          IF (T .EQ. 0) THEN
            IYEAR =0
            M = 0
          ELSE
            IYEAR = INT(( T-1.)/12.)
            IT = INT(T)
            M =  IT - IYEAR*12
          END IF
C
C       SEPERATING THE MODULES FOR THE APPROPRIATE TIME PERIODS
        IF ( T .EQ. 0) THEN
           CALL INITIAL
        ELSE
C          IGUESS IS FOR THE RECYCLING OF PH
           IGUESS = 1
50         CONTINUE
           DO 100 I=1,LAYER
             CALL KINETIC
100        CONTINUE
             CALL OXYGEN
           DO 150 I=1,LAYER
             CALL PYRITE
             CALL TRANSPOR
150       CONTINUE
          IF (IGUESS .NE. 3) THEN
              IGUESS = IGUESS + 1
              GOTO 50
          ENDIF
C
C       EXAMINING WHETHER OR NOT TOTAL DEPLETION HAS OCCURRED
        CC = 0.
        DO 200, I=1,LAYER
           IF (PYR(I,2) .EQ. 0.) THEN
             CC = CC + 1.
           END IF
```

```
200     CONTINUE
        IF ( CC .EQ. LAYER) THEN
          XFLAG = 1
        END IF
C
        END IF
C
      END IF
C
      RETURN
      END
```

```
C FILE 'CONTROL.FOR'
      INCLUDE 'EXEC.FOR'
      INCLUDE 'INPUT.FOR'
      INCLUDE 'SAMPLE.FOR'
      INCLUDE 'SAVE.FOR'
      INCLUDE 'STATS.FOR'
      INCLUDE 'OUTPUT.FOR'
```

```
C FILE 'EXEC.FOR'
C
C     EXECUTIVE MODULE CALLS CONTROL MODULES AND COMPONENT
C     MODULES' CONTROL MODULE, STEPPING THROUGH TIME FOR EACH
C     TRIAL
C
      PROGRAM RATAP
C
      INCLUDE 'IO.INC'
      INCLUDE 'STATS.INC'
      INCLUDE 'COUNTS.INC'
      INCLUDE 'INFO.INC'
      INCLUDE 'OUT.INC'
      INCLUDE 'INPT.INC'
      INCLUDE 'UPDATE.INC'
      INCLUDE 'PARAM.INC'
      INCLUDE 'INTERM.INC'
C
C     CALL INPUT MODULES
C
      CALL INPUT1
      CALL INPUT2
C
C     CALL SAMPLING MODULES
C
      CALL CREATE
      WRITE(SCRUNT,300)
      DO 10 NUMTRL=1,NTRIAL
C
C        SAMPLE NON-TIME-VARIANT INPUT DISTRIBUTIONS
C
         DO 20 I=1,VARN
            CALL CHOOSE(VARNOT(I))
20       CONTINUE
         NTIME=NYEARS+1
         DO 30 IYR = 1,NTIME
C
C           SAMPLE TIME-VARIANT DISTRIBUTIONS
C
            IF(VARY.GE.1)THEN
               DO 40 I=1,VARY
                  CALL CHOOSE(VARIED(I))
40             CONTINUE
            ENDIF
            NEWNT=IYR-1
            T=FLOAT(NEWNT)
            WRITE(SCRUNT,100)NUMTRL,NEWNT
C
C           CALL COMPONENT MODULES
C
            CALL COMEX
C
C           CALL OUTPUT SELECTION ROUTINES
C
            CALL TIMSEL
            CALL SELECT
30       CONTINUE
         CALL SAVEIN
C
C        CALL STATISTICS MODULES
C
         CALL STATS
C
C        CALL OUTPUT MODULES
C
         CALL WRITE
10    CONTINUE
      CALL NAMOUT
      CALL OUTPUT
      WRITE(SCRUNT,300)
      WRITE(SCRUNT,200)
      STOP
100   FORMAT(' TRIAL NUMBER : ',I4,4X,'TIME : ',I5)
200   FORMAT(' RUN COMPLETED')
300   FORMAT(///)
      END
      SUBROUTINE INITIAL
C
C     THE INTIAL CONDITIONS AND INVENTORY ARE CALCULATED IN THIS
C     MODULE
C
C
      INCLUDE 'MODEL.INC'
      INCLUDE 'INTERM.INC'
      REAL HSUM,LSUM
      DIMENSION ID(25)
C
      IF(FLAG1 .EQ. 1.)THEN
        OPEN(5,FILE="INITIAL.OUT")
        WRITE(5,55)
55      FORMAT(' ',"LAYER  MONTH  SOIL TEMP.  WATER CONTENT")
      ENDIF
C
C     THE VALUES;LI AND LSI ARE REAL, THIS STEP CONVERTS THEM TO INT.
      LAYER = INT(LI)
      LAYSAT = INT(LSI)
      MONTH = INT(MNT)
C     LAYSAT IS THE FIRST SATURATED LAYER (IE. IT IS BELOW WATER TAB.)
C     LAYER OF CAPILLARY FRINGE
      LC = LAYSAT
      LSUM = 0.
      HSUM = 0.
      DO 60 II= 1,(LAYSAT-1)
        XCX    = (-HE(LAYSAT-II)-HSUM)/DX(LAYSAT-II)
        ID(II) = ANINT(XCX)
        IF (ID(II) .LE. 0 ) THEN
          GOTO 63
        ELSE
          ID(II) = 1
          HSUM = HSUM + DX(LAYSAT-II)
          LSUM = LSUM + ID(II)
          LC = LAYSAT - LSUM
        END IF
60    CONTINUE
63    CONTINUE
C
      TOTAL=0.0
      DO 64 II=1,(LAYSAT-1)
         TOTAL = DX(II) + TOTAL
64    CONTINUE
      ZWATER = WATTAB - TOTAL
      IF( ABS( ZWATER ).GT. 0.01 )THEN
         CALL ERROR (50,0)
      END IF
      TOTAL = 0.
C
C      GAS CONSTANT
       RR = 82.057E-6
       SUM = 0.
C
C     DO INITIAL CALCULATIONS FOR EVERY LAYER
```

```
C
      IF ( LAYER .GT. 22) THEN
         CALL ERROR (51,0)
      ENDIF
C
      DO 300 I=1,LAYER
C
C     INITIAL CALCULATIONS FOR THE KINETIC MODULE
C
C     DETERMINING THE TEMPERATURE ,MOISTURE CONTENT AND INFILTRATION RATE
C     AS A FUNCTION OF DEPTH
C
      DO 70 MM =1,12
C
C        TEMPERATURE
         W = 2.*3.14/12.
         IF ( MM .EQ. 1) THEN
C
C    SUM IS THE DISTANCE FROM THE SURFACE DOWN TO THE LOWER BOUNDRY
C         OF THE LAYER
C
           SUM  = SUM + DX(I)
           Z(I) = SUM
         ENDIF
C
         MT = MM - 4
         IF (MT .EQ. -3) THEN
           MT = 9
         ELSE IF (MT .EQ. -2) THEN
           MT = 10
         ELSE IF (MT .EQ. -1) THEN
           MT = 11
         ELSE IF (MT .EQ. 0) THEN
           MT = 12
         END IF
C
         TS(I,MM) = AVGTEM +
    &                COEFA0*(SIN(W*MT-COEFPS*W
    &                -Z(I)/COEFDD))*(EXP(-Z(I)/COEFDD))
C
C        INFILTRATION RATE
C
C        DEEP ZONE INFILTRATION
         IF (I .EQ. LAYSAT+1) THEN
             INFILT(I,MM) = VR(MM)*VRFRAC
             VRAIN(I,MM) = INFILT(I,MM)*ATAIL*1000.
         ELSE
C        NON-DEEP ZONE INFILTRATION
C        NOTE THAT I=25 IS A REFERENCE DEPTH
           INFILT(25,MM) = VR(MM)*1.0
           INFILT(I,MM) = VR(MM)*1.0
           VRAIN(I,MM) = INFILT(I,MM)*ATAIL*1000.
           VRAIN(25,MM) = INFILT(25,MM)*ATAIL*1000.
        ENDIF
C
```

```
C        POROSITIES
         IF ( I .LT. LC) THEN
C
C     H(I) IS THE HEIGHT OF THE LAYERS UPPER BOUNDRY ABOVE WATER TABLE
C
           H(I) = WATTAB - (SUM - DX(I) )
           CC1 = -HE(I)/H(I)
           CC2 = CC1**LA(I)
           NW(I) = CC2*(NT(I)*NR(I)) + NR(I)
           IF (NW(I) .GT. NT(I) ) THEN
              NW(I) = NT(I)
           ENDIF
         ELSE
           NW(I) = NT(I)
         END IF
C
           S(I) = NW(I)/NT(I)
           NA(I) = NT(I)-NW(I)
C
       IF(FLAG1 .EQ. 1.)THEN
         WRITE(5,105) I,MM,TS(I,MM),NW(I)
105      FORMAT(' ',1X,I3,3X,I3,3X,E10.4,3X,E10.4)
       ENDIF
C
70       CONTINUE
C
         DO 125 J =1,3
C
C        INITIAL CALCULATIONS FOR THE PYRITE MODULE
C
C        CALCULATE THE INITIAL PYRITE SURFACE AREA
           VT(I) = ATAIL*DX(I)
           RAD(I,J) = RADMAX
           ALPHAP(I,J) = 7.128E4*XPYR
           IF( RADMAX .EQ. 0. )THEN
                SA(I,J) = 0.0
           ELSE
                SA(I,J) = 3./(MOLARD*RADMAX)
           END IF
           AS(I,J) = ALPHAP(I,J)*VT(I)
C
C       INITIAL CALCULATIONS FOR THE SPECIATION MODULE
C
C        CONCENTRATIONS
C          COX IS OXYGEN CONC. IN MOL/M3
           COX(I,J) = 8.9
           P(I,J) = 2.3
C          OXYGEN SET BELOW ATM TO APPROXIMATE MEAN VALUE
           PO2(I,J) = 5.0
C
C     INITIALIZING CALCULATIONS FOR THE ION TRANSPORT MODULE
C
C     INITIALIZING
         AFLUX(I,J) = 0.
         KC(I,J) = 0.
```

```
            R1(I,J) = 0.
            R2(I,J) = 0.
            RO2(I,J) = 0.
            R1B(I,J) = 0.
            NP(I,J) = 0.
            HCO3(I,J) = 0.
            SULF(I,J) = 0.
            ALUM(I,J) = 0.
            IRON(I,J) = 0.
            CTT(I,J) = 0.
            ATOTAL(I,J) = 0.
            AYEAR(I,J) = 0.
C       MOLES/M3 TAILINGS
            PYR(I,J) = BULKD*XPYR/120.
        IF ( I .LE. COVER) THEN
            PYR(I,J) = 0.
        ENDIF
             GYP(I,J) = BULKD*XGYP/136.
             CACO3(I,J) = BULKD*XCACO3/100.
             FEOH3(I,J) = BULKD*XFEOH3/74.9
             ALOH3(I,J) = BULKD*XALOH3/46.0
             SER(I,J) =   BULKD*XSER/371.37
C       MOLES/L
             CA(I,J) =    (KCASO4/F(2)**2.)**(0.5)
             FE2(I,J) =   1.E-8
             SO4(I,J) =   (KCASO4/F(2)**2.)**(0.5)
             SO4T(I,J)=   SO4(I,J)
             FE2T(I,J)=   1.E-6
             CAT(I,J) =   CA(I,J)
             ALT(I,J) =   1.E-10
             FE3T(I,J) =  1.E-6
             POTAS(I,J) = 1.E-4
             CT(I,J) = 0.001
             NO3T(I,J) = 0.0
             FE3(I,J) =  1.E-6
             AL3(I,J) =  1.E-10
C
C       WHEN CACO3 IS PRESENT THE CO2 LEVEL RISES
             IF (CACO3(I,1) .GT. 0.) THEN
                PCO2(I,J) = 3.2E-4*100.
             ELSE
                PCO2(I,J) = 3.2E-4
             ENDIF
C
C         INITIALIZING THE SYSTEM PH
C         (THIS VALUE IS EMPLOYED IN THE PYRITE MODULE)
C
C         ADJUSTING THE INITIAL GUESS IF A "CASE" CHANGE OCCURS
C           WHEN CALCITE IS PRESENT
C           CASES 1.11,1.12,1.13, AND 1.14
C
            IF (CACO3(I,2) .GT. 0.) THEN
              PH(I,3) = 6.5
C
C           WHEN CALCITE IS ABSENT
```

```
C
C            CASES 2.1,2.2,3.1,AND 3.2
             ELSE   IF (ALOH3(I,2) .GT. 0.) THEN
                      PH(I,3) = 4.0
C
C            CASE 410 OR 510
             ELSE
                     PH(I,3) = 2.0
             ENDIF
125         CONTINUE
C
300      CONTINUE
C
C
C        CONCENTRATIONS IN RAINWATER
C        I=25 IS USED AS A REFERENCE DEPTH
         DO 400 J =1,3
           FE2T(25,J) = 0.0
           CAT(25,J) =  1.E-4
           SO4T(25,J) = 1.E-6
           FE3T(25,J) = 0.0
           ALT(25,J) = 0.0
           CTT(25,J) = 1.E-5
           CT(25,J) = 1.E-5
           NO3T(25,J) = 1.E-5
           POTAS(25,J) = 1.E-5
400      CONTINUE
C
         RETURN
         END
```

```
C FILE 'INPUT.FOR'
C
      SUBROUTINE INPUT1
C
C      THE FOLLOWING SUBROUTINE INPUTS THE FILE CONTAINING THE
C      PROBABILISTIC PARAMATER DESCRIPTIONS AND ALLOWS THE USER
C      TO SAVE INPUTS TO KEY AND DETAILED RESULTS FILES
C
      INCLUDE 'IO.INC'
      INCLUDE 'COUNTS.INC'
      INCLUDE 'PARAM.INC'
      CHARACTER*12 FNAME
      CHARACTER*6 CORNAM
      CHARACTER*1 TVARY(300)
      INTEGER*2 REG,ARB,NCORR
      SCRUNT=0
      FUNIT1=1
      FUNIT2=2
      FUNIT=4
      CALL UNDERO('T')
      WRITE(SCRUNT,1000)
      CALL FILER(SCRUNT)
C
C     OPEN FIRST INPUT FILE
C
      WRITE (SCRUNT,1250)
      READ (SCRUNT,1400) FNAME
      WRITE (SCRUNT,1350) FNAME
      OPEN (FUNIT,FILE=FNAME,STATUS='OLD',IOSTAT=IERR)
      IF (IERR.NE.0) CALL ERROR (29,0)
      ILINE=1
      READ (FUNIT,1400,END=998,ERR=996) TITLE
C
C     OPEN OUTPUT FILE(S)
C
      ILINE=ILINE+1
      READ (FUNIT,1410,END=998,ERR=996) FSAVE,SKEWFG
      ILINE=ILINE+1
      READ (FUNIT,1400,END=998,ERR=996) FNAME
      IF (FSAVE.EQ.'Y') THEN
C
C        OPEN DETAILED RESULTS FILE
C
         WRITE (SCRUNT,1350) FNAME
         OPEN (FUNIT1,FILE=FNAME,STATUS='NEW',IOSTAT=IERR)
         IF (IERR.NE.0) THEN
            CALL ERROR (102,0)
            OPEN (FUNIT1,FILE=FNAME)
         ENDIF
      ENDIF
      ILINE=ILINE+1
      READ (FUNIT,1400,END=998,ERR=996) FNAME
C
C     OPEN KEY FILE
C
```

```
      WRITE (SCRUNT,1350) FNAME
      OPEN (FUNIT2,FILE=FNAME,STATUS='NEW',IOSTAT=IERR)
      IF (IERR.NE.0) THEN
         CALL ERROR (102,0)
         OPEN (FUNIT2,FILE=FNAME)
      ENDIF
C
C     READ COUNTERS AND CHECK TIME
C
      ILINE=ILINE+1
      READ (FUNIT,1450,END=998,ERR=996) NPARM,NARB,NCORR
      ILINE=ILINE+1
      READ (FUNIT,1550,END=998,ERR=996) NSTART,NTRIAL
      ILINE=ILINE+1
      READ (FUNIT,1460,END=998,ERR=996) RYEARS
      NYEARS=INT(RYEARS)
      NYR=NYEARS/12
      DT=1.0
      NDT=1
      IF(12*NYR.LT.NYEARS)NYR=NYR+1
      NFILE=0
      VARY=0
      VARN=0
      VARYF=0
      REG=NPARM-(NCORR+NARB)
      ARB=NPARM-NCORR
      DO 1050 I=1,NPARM
         IF (I.LE.REG) THEN
C
C           READ REGULAR DISTRIBUTIONS
C
            ILINE=ILINE+1
            READ(FUNIT,1500,END=999,ERR=996)VARTIT(I),EFLAG(I),NTYPE(I),
     &         TVARY(I),P1(I),P2(I),P3(I),P4(I)
            IF (NTYPE(I).EQ.2) THEN
               IF (P4(I).LE.P3(I)) CALL ERROR (31,ILINE)
            ELSEIF (NTYPE(I).EQ.3) THEN
               IF(P4(I).LE.P3(I)) CALL ERROR (30,ILINE)
            ELSEIF (NTYPE(I).EQ.6) THEN
               IF(P3(I).LE.P1(I)) CALL ERROR (33,ILINE)
            ELSEIF (NTYPE(I).EQ.8) THEN
               IF(P2(I).LE.P1(I).OR.P3(I).LE.0.0.OR.P4(I).LE.0.0) CALL
     &            ERROR (34,ILINE)
            ELSEIF (NTYPE(I).EQ.9.OR.NTYPE(I).EQ.10) THEN
               CALL ERROR (6,ILINE)
            ELSEIF (NTYPE(I).NE.1.AND.NTYPE(I).NE.4.AND.NTYPE(I).NE.5
     &         .AND.NTYPE(I).NE.7) THEN
               CALL ERROR (12,ILINE)
            ENDIF
         ELSEIF (I.LE.ARB) THEN
C
C           READ ARBITRARY DISTRIBUTIONS
C
            ILINE=ILINE+1
            READ(FUNIT,1610,END=999,ERR=996)VARTIT(I),EFLAG(I),NTYPE(I),
     &         TVARY(I),NACELL(I),P1(I),P2(I),(V(I,I2),I2=1,NACELL(I))
            IF (NTYPE(I).NE.9) CALL ERROR (8,ILINE)
         ELSE
C
C           READ CORRELATED DISTRIBUTIONS
C
            ILINE=ILINE+1
            READ(FUNIT,1600,END=999,ERR=996)VARTIT(I),EFLAG(I),NTYPE(I),
     &         TVARY(I),CORNAM,P1(I),P2(I),P3(I),P4(I),P5(I)
            IF (NTYPE(I).NE.10) CALL ERROR (7,ILINE)
            K=1
10          IF (VARTIT(K).EQ.CORNAM) THEN
               IF (TVARY(K).NE.'V'.OR.(TVARY(K).EQ.'V'.AND.TVARY(I).EQ.
     &            'V')) THEN
                  CORNUM(I)=K
               ELSE
                  CALL ERROR (18,ILINE)
               ENDIF
            ELSEIF (K.LT.I) THEN
               K=K+1
               GOTO 10
            ELSE
               CALL ERROR (4,ILINE)
            ENDIF
         ENDIF
         IF (TVARY(I).EQ.'V') THEN
            VARY=VARY+1
            VARIED(VARY)=I
            IF (EFLAG(I).EQ.'F') VARYF=VARYF+1
         ELSE
            VARN=VARN+1
            VARNOT(VARN)=I
            IF (EFLAG(I).EQ.'F') NFILE=NFILE+1
         ENDIF
1050  CONTINUE
      CLOSE (FUNIT)
      RETURN
996   CALL ERROR (3,ILINE)
998   CALL ERROR (5,ILINE)
999   CALL ERROR (9,ILINE)
1000  FORMAT (' RATAP',/)
1250  FORMAT (/,' First Input File Name? ')
1350  FORMAT (' Opening File : ',A12)
1400  FORMAT (A)
1410  FORMAT (A1,1X,A1)
1450  FORMAT (3I4)
1460  FORMAT (2E7.2)
1500  FORMAT (A6,1X,A1,1X,I2,1X,A1,4E11.6)
1550  FORMAT (I10,I4)
1600  FORMAT (A6,1X,A1,1X,I2,1X,A1,1X,A6,5E11.6)
1610  FORMAT (A6,1X,A1,1X,I2,1X,A1,I3,2E11.6,25(F6.2))
      END
C
C
C
```

```
      SUBROUTINE INPUT2
C
C     SUBROUTINE PROMPTS FOR INPUT FILE AND READS INPUT INFORMATION
C     SPECIFIC TO RATAP
      INCLUDE 'IO.INC'
      INCLUDE 'COUNTS.INC'
      INCLUDE 'INFO.INC'
      CHARACTER*12 FNAME
C
C     OPEN SECOND INPUT FILE
C
      WRITE (SCRUNT,700)
      READ (SCRUNT,810) FNAME
      WRITE (SCRUNT,820) FNAME
      OPEN (FUNIT,FILE=FNAME,STATUS='OLD',IOSTAT=IERR)
      IF (IERR.NE.0) CALL ERROR(29,0)
C
C     READ OUTPUT PARAMETER SPECIFICATIONS
C
      NVARYF=0
C
C     READ TIME STEPS TO BE SAVED
C
      ILINE=ILINE+1
      READ (FUNIT,900,END=999,ERR=996) NSTEPF
      IF (NSTEPF.GT.0) THEN
         ILINE=ILINE+1
         READ (FUNIT,920,END=999,ERR=996) (TFILE(I),I=1,NSTEPF)
         NTEST=-1
         DO 52 I=1,NSTEPF
            IF (NTEST.GE.TFILE(I)) CALL ERROR (11,ILINE)
            NTEST=TFILE(I)
52       CONTINUE
      ELSE
         ILINE=ILINE+1
         READ (FUNIT,810,END=999,ERR=996)
      ENDIF
C
C     READ OUTPUT PARAMETERS
C
      ILINE=ILINE+1
      READ (FUNIT,900,ERR=996) NARRAY
      J=1
      DO 10 I=1,NARRAY
         ILINE=ILINE+1
         READ (FUNIT,940,END=999,ERR=996) VARNAM(I),NVAR(I)
         IF (NVAR(I).GT.0) THEN
            NVARYF=NVARYF+NVAR(I)
            KK=NVAR(I)
            DO 20 K=1,KK
               ILINE=ILINE+1
               READ (FUNIT,950,END=999,ERR=996) LOC(J)
               J=J+1
20          CONTINUE
         ENDIF
```

```
10    CONTINUE
      NARRAY=I-1
      IFILE=(NVARYF+VARYF)*NSTEPF*NYR+NFILE
      IF (IFILE.GT.750) CALL ERROR (28,ILINE)
      CLOSE(FUNIT)
      RETURN
996   CALL ERROR (3,ILINE)
999   CALL ERROR (5,ILINE)
700   FORMAT (/,' Second Input File Name? ')
810   FORMAT (A)
820   FORMAT (' Opening File : ',A12)
900   FORMAT (I3)
920   FORMAT (12(I3))
940   FORMAT (A6,I3)
950   FORMAT (4X,I3)
      END
C
C
C
      SUBROUTINE ERROR (I,ILINE)
C
C     SUBROUTINE GENERATES ERROR AND WARNING MESSAGES.  ALL ERRORS
C     TERMINATE THE PROGRAM.  WARNINGS ASK IF EXECUTION IS TO BE STOPPED
C     OR CONTINUED.
C
      INCLUDE 'IO.INC'
      CHARACTER*1 Q
      WRITE (SCRUNT,300)
      IF (I.LE.100) THEN
C
C        GENERATE ERROR MESSAGES
C
         WRITE (SCRUNT,300) ' ***************  ERROR  ***************'
         IF (I.EQ.1) THEN
            WRITE (SCRUNT,300) ' (001)'
         ELSEIF (I.EQ.3) THEN
            WRITE (SCRUNT,300) ' (003) ERROR IN INPUT FILE'
         ELSEIF (I.EQ.4) THEN
            WRITE (SCRUNT,300) ' (004) CORRELATED NAME NOT FOUND'
         ELSEIF (I.EQ.5) THEN
            WRITE (SCRUNT,300) ' (005) UNEXPECTED END OF DATA'
         ELSEIF (I.EQ.6) THEN
            WRITE (SCRUNT,300) ' (006) TYPE ERROR IN REGULAR DIST''ns'
         ELSEIF (I.EQ.7) THEN
            WRITE (SCRUNT,300) ' (007) TYPE ERROR IN CORRELATED DIST''ns
     &'
         ELSEIF (I.EQ.8) THEN
            WRITE (SCRUNT,300) ' (008) TYPE ERROR IN ARBITRARY DIST''ns'
         ELSEIF (I.EQ.9) THEN
            WRITE (SCRUNT,300) ' (009) NUMBER OF PARAMETERS INCORRECT'
         ELSEIF (I.EQ.11) THEN
            WRITE (SCRUNT,300) ' (011) TIME STEPS MUST INCREASE'
         ELSEIF (I.EQ.12) THEN
            WRITE (SCRUNT,300) ' (012) DISTRIBUTION NUMBER NOT DEFINED'
         ELSEIF (I.EQ.18) THEN
```

```
            WRITE (SCRUNT,300) ' (018) CANNOT CORRELATE PARAMETERS'
         ELSEIF (I.EQ.28) THEN
            WRITE (SCRUNT,300) ' (028) TOO MANY OUTPUTS'
         ELSEIF (I.EQ.29) THEN
            WRITE (SCRUNT,300) ' (029) FILE NOT FOUND'
         ELSEIF (I.EQ.30) THEN
            WRITE (SCRUNT,300) ' (030) ERROR IN LOGNORMAL SPECIFIERS'
         ELSEIF (I.EQ.31) THEN
            WRITE (SCRUNT,300) ' (031) ERROR IN NORMAL SPECIFIERS'
         ELSEIF (I.EQ.32) THEN
            WRITE (SCRUNT,300) ' (032) TIME MUST BE IN WHOLE NUMBERS'
         ELSEIF (I.EQ.33) THEN
            WRITE (SCRUNT,300) ' (033) ERROR IN TRIANGULAR SPECIFIERS'
         ELSEIF (I.EQ.34) THEN
            WRITE (SCRUNT,300) ' (034) ERROR IN BETA SPECIFIERS'
         ELSEIF (I.EQ.35) THEN
            WRITE (SCRUNT,300) ' (035)'
         ELSEIF (I.EQ.50) THEN
            WRITE (SCRUNT,300) ' (050) ERROR IN THE VALUE INPUT FOR WATT
     &AB OR LAYSAT'
         ELSEIF (I.EQ.51) THEN
            WRITE (SCRUNT,300) ' (051) UNACCEPTABLE NUMBER OF LAYERS'
         ELSEIF (I.EQ.52) THEN
            WRITE (SCRUNT,300) ' (052) CALCULATED PH LESS THAN ZERO'
         ELSEIF (I.EQ.53) THEN
            WRITE(SCRUNT,300) ' (053) MAXIMUM NUMBER OF ITERATIONS HAS B
     &EEN EXCEEDED'
         ELSE
            WRITE (SCRUNT,300) ' ERROR NUMBER NOT DEFINED'
         ENDIF
      ELSE
C
C        GENERATE WARNING MESSAGES
C
         WRITE (SCRUNT,300) ' ***************  WARNING  ***************'
         IF (I.EQ.101) THEN
            WRITE (SCRUNT,300) ' (101)'
         ELSEIF (I.EQ.102) THEN
            WRITE (SCRUNT,300) ' (102) ABOUT TO OVER WRITE EXISTING FILE
     &'
         ENDIF
         WRITE (SCRUNT,300) '  - OK TO CONTINUE (Y/N)? '
         READ (SCRUNT,300) Q
         IF (Q.EQ.'Y'.OR.Q.EQ.'y') THEN
C
C           RESUME EXECTION
C
            WRITE (SCRUNT,300) ' RESUMING EXECUTION'
            RETURN
         ENDIF
      ENDIF
C
C     STOP PROGRAM
C
      WRITE (SCRUNT,300) ' PROGRAM TERMINATED'
      WRITE (SCRUNT,320) ILINE
      WRITE (SCRUNT,300) ' SEE USERS MANUAL APPENDIX A'
      STOP
300   FORMAT (A)
310   FORMAT (A37,I3)
320   FORMAT (' LAST LINE READ =',I4)
      END
```

```
C FILE 'INTERM.INC'
      CHARACTER*4 C111,C112,C121,C122,C210,C220,C310,C320,C410,
     &C420,C510,C520,CASE(25)
      REAL*4 PH(25,3),PCO2(25,3),PO2(25,3),P(25,3),KC(25,12),R1(25,3),
     &R2(25,3),TS(25,13),NW(25),RO2(25,3),AS(25,3),PYR(25,3),FE3(25,3),
     &SA(25,3),ALPHAP(25,3),RAD(25,3),NA(25),R1B(25,3),S(25),AL3(25,3),
     &NP(25,3),VT(25),COX(25,3),VRAIN(25,12),Z(25),H(25),FE2(25,3)
     &,CT(25,3),CA(25,3),HCO3(25,3),BICARBP(25,3),SULF(25,3),FE3T(25,3),
     &ALUM(25,3),IRON(25,3),FEITY,ALITY,SFACT,FET,CO,SO4T(25,3),
     &CONTS,RT(25,2),SUM,POTAS(25,3),CAEQ(25),TOT(25,3),FE2T(25,3),
     &CAT(25,3),SO4(25,3),ALFACT,FEFACT,ALT(25,3),CACO3(25,3),CW(25),
     &FEOH3(25,3),ALOH3(25,3),SER(25,3),GYP(25,3),INFILT(25,12),
     &DELCAL(25),XCT(25),CTT(25,3),NO3T(25,3),SULFP(25,3),CON1,
     &DGYP(25,3),CALIN,AFLUX(25,3),RPYR(25),XFLAG,FPH,
     &BLANK1(25,3),BLANK2(25,3),BLANK3(25,3),BLANK4(25,3),BLANK5(25,3),
     &FRAC,RSER(25),ATOTAL(25,3) ,AYEAR(25,3)
      INTEGER I,NN,M,LC,LAYER,LAYSAT,II,IGUESS,MONTH
      COMMON /INTERM/ PH,PCO2,PO2,P,KC,R1,R1B,R2,RO2,AS,PYR,SA,ALPHAP,
     &RAD,NA,S,NP,I,VT,NW,TS,NN,M,COX,RR,LC,LAYER,LAYSAT,VRAIN,Z,H,CT,
     &CA,HCO3,BICARBP,FE3,AL3,SULF,ALUM,CASE,C111,C121,C112,C122,C210,
     &C220,C310,C320,C410,C420,C510,C520,IRON,FEITY,ALITY,SFACT,SO4,XCT,
     &FET,CONTS,RT,FE2,SUM,POTAS,CAEQ,TOT,CO,FE2T,CAT,SO4T,ALFACT,
     &FEFACT,ALT,FE3T,CACO3,FEOH3,ALOH3,SER,GYP,INFILT,DELCAL,II,CW,
     &CTT,NO3T,SULFP,CON1,PCASE,RG,DGYP,CALIN,AFLUX,RPYR,XFLAG,FPH,
     &BLANK1,BLANK2,BLANK3,BLANK4,BLANK5,IGUESS,FRAC,RSER,ATOTAL,AYEAR
     &,MONTH
```

```
      SUBROUTINE KINETIC
C
C     KINETICS MODEL; BIOLOGICAL AND CHEMICAL RATES OF REACTION
C
      INCLUDE 'INTERM.INC'
      INCLUDE 'MODEL.INC'
      DIMENSION U(25,3),RTR(25)
      REAL  LIMP
C
C
      IF (FLAG2 .EQ. 1. .AND. I .EQ. 1. .AND. T .EQ. 1. .AND. IGUESS
     &.EQ. 3) THEN
         OPEN(6,FILE='KINETIC.OUT')
         WRITE(6,75)
75       FORMAT(' ',4X,"T",5X,"LAYER",2X,"R1(I,2)",3X,"R2(I,2)",4X,
     &"RO2(I,2)",4X,"NW(I)",5X,"TS(I,M)",4X,"PH(I,3)",4X,"PCO2(I,3)")
      END IF
C
C     CONSTANTS
      RG = 1.987
C
C     CALCULATING THE BIOLOGICAL REACTION RATE
C
C        CALCULATING THE CONSTANT
         TERM1 = EXP(BIOEA/(1.987*303.))
         TERM2 = 1.+10**(2.5-3.25) + 10**(3.25-4.0)
         TERM3 = 1./(2.3/(2.3+1.29E-3) *1.3*3.2E-4/(1.E-4+3.2E-4) *1.0)
         CONST = LOG( TERM1*TERM2*TERM3 )
C
C       MAXIMUM TEMPERATURE LIMITATIONS
        IF (TS(I,M) .GT. 303.)  THEN
           TEMP = 303.
        ELSE
           TEMP = TS(I,M)
        ENDIF
C
        U1 = BIOMAX*EXP(CONST)*EXP(-BIOEA/(RG*TEMP))
        U2 = 1/(1+10**(2.5-PH(I,3))+ 10**(PH(I,3)-4.0))
        U3 = S(I)*P(I,3)/(LIMP +P(I,3))
        U4 = 1.3*PCO2(I,3)/(10**(-4.0)+PCO2(I,3))
        U(I,2) = U1*U2*U3*U4
C
C       IF FREEZING OCCURS THE BIOLOGICAL RATE IS SET EQUAL TO ZERO
        IF ( TS(I,M) .LE. 273.) THEN
          U(I,2) = 0.
        ENDIF
C
C       BIOLOGICAL SPECIFIC REACTION RATE
        R1(I,2) = -U(I,2)*BIOXP/BIOYXS
C
C       CALCULATING THE CHEMICAL REACTION RATE
C
C       EFFECT OF PH ON CHEMICAL RATE
        FPH = 0.25*(PH(I,3))**(0.70)
C
```

```
          KC(I,M) = CHEMKC*EXP(-CHEMEA/(RG*TS(I,M)))
C
C         IF THE WATER CONTENT GO TO ZERO KC  IS SET EQUAL TO ZERO
          IF ( NW(I) .EQ. 0.0) THEN
            KC(I,M) = 0
          END IF
C
C         CHEMICAL SPECIFIC REATION RATE
          R2(I,2) = -FPH*KC(I,M)*PO2(I,3)
C
C         TOTAL RATE (NOT INCLUDING OXYGEN EFFECT ON BIO.)
          RTR(I) = R1(I,2) + R2(I,2)
C
C         RATE OF OXYGEN DEPLETION (MOL.M-3.MTH-1)
C
          IF ( NA(I) .GT. 0) THEN
C            MOLES/(M3 AIR MTH)
             RO2(I,2) = 3.75*(RTR(I))*ALPHAP(I,3)/NA(I)
          ELSE
C            MOLES/(M3 WATER MTH)
             RO2(I,2) = 3.75*RTR(I)*ALPHAP(I,3)/NW(I)
          END IF
C
C         IF NO PYRITE WAS PRESENT IN A LAYER THEN THE RATES ARE
C         SET TO ZERO
C
          IF (PYR(I,3) .EQ. 0) THEN
              R1(I,2) =0.
              R2(I,2) =0.
              RO2(I,2) = 0.
          END IF
C
         IF ( M .EQ. MONTH .AND. FLAG2 .EQ. 1. .AND. IGUESS .EQ. 3)THEN
             WRITE(6,150) T,I,R1(I,2),R2(I,2),RO2(I,2),NW(I),TS(I,M),
     &       PH(I,3),PCO2(I,3)
150          FORMAT(' ',E10.2,1X,I3,7(1X,E10.4))
         ENDIF
C
C
          RETURN
          END
```

```
C FILE 'MODEL.INC'
C COMMON BLOCK FOR INPUT DATA SET

      REAL*4 BIOEA,CHEMEA,BIOMAX,LIMP,BIOXP,BIOYXS,LIMO2,MOLARD,ALPHA,
     &HENRY,KCO2,COEFAO,AVGTEM,COEFPS,BETA,RADMAX,DX(22),CHEMKC,
     &VR(12),LI,COVER,LSI,COEFDD,CHSO4,CCASO4,CALSO4,CFEOH,CFEOH2,
     &CFEOH3,CALOH3,F(3),CFESO4,COEFX,COEFY,VRFRAC,
     &KCASO4,DK1,DK2,KCACO3,NR(22),NT(22),HE(22),WATTAB,
     &LA(22),KFEOOH,CALOH2,CALOH,KBAS,COEFAL,XGYP,XPYR,BULKD,
     &FLAG1,FLAG2,FLAG3,FLAG4,FLAG5,FLAG6,MNT
      COMMON /INPT/ FLAG1,FLAG2,FLAG3,FLAG4,FLAG5,
     &FLAG6,MNT,
     &BIOEA,CHEMEA,BIOMAX,LIMP,BIOXP,BIOYXS,LIMO2,XKFE3,XPYR,XGYP,
     &XFEOH3,XALOH3,XSER,XCACO3,SATCT,BULKD,ATAIL,MOLARD,ALPHA,BETA,
     &COEFX,COEFY,RADMAX,CHEMKC,COEFAL,LI,COVER,LSI,HENRY,KCO2,COEFAO,
     &AVGTEM,COEFPS,COEFDD,WATTAB,VRFRAC,LA,NT,NR,HE,
     &DX,VR,CHSO4,CCASO4,
     &CALSO4,CFEOH,CFEOH2,CFESO4,
     &CFEOH3,CALOH3,F,KCASO4,
     &DK1,DK2,KCACO3,KFEOOH,CALOH2,CALOH,KBAS

      INTEGER*4 NYEARS,NEWNT,NYR
      INTEGER*2 NUMTRL, NTRIAL,NDT
      REAL*4 T,RYEARS,DT
      COMMON /TIME/ T, NUMTRL, NTRIAL,NYEARS, NDT,RYEARS,DT,NEWNT,NYR
```

```
C FILE 'OUTPUT.FOR'
C
      SUBROUTINE WRITE
C
C     WRITES VALUES CONTAINED IN 'XOUT' (SAMPLED INPUTS AND
C     CALCULATED PARAMETERS) TO DETAILED RESULTS FILE (UNIT 1)
C
      INCLUDE 'OUT.INC'
      INCLUDE 'IO.INC'
      INCLUDE 'COUNTS.INC'
      IF (FSAVE.EQ.'Y'.AND.NOUT.GT.0) THEN
         IF (NUMTRL.EQ.1) CALL FILER (FUNIT1)
         WRITE (FUNIT1,900) (XOUT(I),I=1,NOUT)
      ENDIF
      RETURN
900   FORMAT (5(150(1X,E9.3)))
      END
C
C
C
      SUBROUTINE NAMOUT
C
C     ASSIGNS VARIABLE NAMES AND LOCATION AND SUBSTANCE CODES TO
C     CHARACTER VARIABLES FOR OUTPUT IN KEY FILE
C
      INCLUDE 'IO.INC'
      INCLUDE 'INFO.INC'
      INCLUDE 'COUNTS.INC'
      KF=1
C
C     WRITE SAMPLED INPUT VARIABLE NAMES FOR KEY
C     FILE FOR NON-TIME-VARIANT DISTRIBUTIONS
C
      DO 10 I=1,VARN
         IF (EFLAG(VARNOT(I)).EQ.'F') THEN
            WRITE (NAMEF(KF),100) VARTIT(VARNOT(I))
            KF=KF+1
         ENDIF
 10   CONTINUE
      JJ=1
C
C     WRITE SAMPLED INPUT VARIABLE NAMES FOR KEY
C     FILE FOR TIME-VARIANT DISTRIBUTIONS
C
      IF (VARY.GE.1) THEN
         DO 60 I=1,VARY
            IF (EFLAG(VARIED(I)).EQ.'F') THEN
               DO 85 K=1,NYR
                  DO 80 J=1,NSTEPF
                     WRITE (NAMEF(KF),150) VARTIT(VARIED(I)),K,TFILE(J)
                     KF=KF+1
80                CONTINUE
85             CONTINUE
            ENDIF
60       CONTINUE
```

```
      ENDIF
C
C     WRITE OUTPUT VARIABLE NAMES FOR KEY FILE.
C     NAMES INCLUDE VARIABLE NAME, SUBSTANCE, LOCATION, AND TIME.
C
      DO 20 I=1,NARRAY
         IF (NVAR(I).GT.0) THEN
            DO 30 J=1,NVAR(I)
               DO 55 L=1,NYR
                  DO 50 K=1,NSTEPF
                     WRITE (NAMEF(KF),200) VARNAM(I),LOC(JJ),L,TFILE(K)
                     KF=KF+1
 50               CONTINUE
 55            CONTINUE
               JJ=JJ+1
 30         CONTINUE
         ENDIF
 20   CONTINUE
 100  FORMAT (2X,A6)
 150  FORMAT (2X,A6,16X,2I6)
 200  FORMAT (2X,A6,11X,I2,3X,2I6)
      RETURN
      END
C
C
C
      SUBROUTINE OUTPUT
C
C     SUBROUTINE WRITES SUMMARY STATISTISTICS AND VARIABLE NAMES TO
C     A 'KEY' FILE (UNIT2)
C
      INCLUDE 'IO.INC'
      INCLUDE 'STATS.INC'
      INCLUDE 'COUNTS.INC'
      CHARACTER*9 VECTOR(5)
C
C     WRITE TO KEY FILE
C
      IF (NOUT.GT.0) THEN
         CALL FILER (FUNIT2)
         WRITE (FUNIT2,900) TITLE
         WRITE (FUNIT2,930) NTRIAL
         IF(SKEWFG.EQ.'Y')THEN
            WRITE(FUNIT2,910)
         ELSE
            WRITE(FUNIT2,915)
         ENDIF
         DO 20 I=1,NOUT
            DO 30 J=1,5
               VECTOR(J)='         '
 30         CONTINUE
            IF(SDEV(I).NE.-999.)THEN
               WRITE(VECTOR(1),800)SDEV(I)
               IF(SKEWFG.EQ.'Y'.AND.SKEW(I).NE.-999.)THEN
                  WRITE(VECTOR(4),800)SKEW(I)
                  IF(KURT(I).NE.-999.)
     &               WRITE(VECTOR(5),800)KURT(I)
               ENDIF
            ENDIF
            IF(GMEAN(I).NE.-999.)THEN
               WRITE(VECTOR(2),800)GMEAN(I)
               IF(GSDEV(I).NE.-999.)THEN
                  WRITE(VECTOR(3),800)GSDEV(I)
               ENDIF
            ENDIF
            WRITE(FUNIT2,850)I,NAMEF(I),S1(I),(VECTOR(J),J=1,3),XMIN(I),
     &         XMAX(I),(VECTOR(J),J=4,5)
20       CONTINUE
      ENDIF
      CLOSE (FUNIT1)
      CLOSE (FUNIT2)
850   FORMAT(I3,2X,A36,3X,E9.3,3(2X,A9),2(2X,E9.3),2(2X,A9))
800   FORMAT(E9.3)
900   FORMAT (1X,A40)
910   FORMAT (5X,'PARAMETER',7X,'LOCATION',2X,'YEAR',1X,'MONTH',4X,
     &   'MEAN',6X,'STD DEV',3X,'GEOM MEAN',3X,'GEOM SD',
     &   4X,'MINIMUM',4X,'MAXIMUM',4X,'SKEWNESS',3X,'KURTOSIS')
915   FORMAT (5X,'PARAMETER',7X,'LOCATION',2X,'YEAR',1X,'MONTH',4X,
     &   'MEAN',6X,'STD DEV',3X,'GEOM MEAN',3X,'GEOM SD',
     &   4X,'MINIMUM',4X,'MAXIMUM')
930   FORMAT (1X,'NUMBER OF TRIALS: ',I5)
      RETURN
      END
C
C
C
      SUBROUTINE FILER(UNIT)
C
C     WRITES DATE AND TIME TO TOP OF OUTPUT FILES
C
      INTEGER*2 UNIT
      CHARACTER*8 DAY, HOUR
      CALL DATE(DAY)
      CALL TIME(HOUR)
      IF(UNIT.NE.0)THEN
         WRITE(UNIT,100)DAY,HOUR
      ELSE
         WRITE(UNIT,200)DAY,HOUR
      ENDIF
      RETURN
100   FORMAT('FILE CREATED ',A8,' AT ',A8)
200   FORMAT(' RUN STARTED ',A8,' AT ',A8)
      END
      SUBROUTINE OXYGEN
C
C     OXYGEN MODEL; DIFFUSION AND ADVECTION
C
      INCLUDE 'INTERM.INC'
      INCLUDE 'MODEL.INC'
C
      DIMENSION DE(25),KB(25),R(25),UR(25),W(25),CONT1(25),
    & CONT2(25),C(25),A(25,3)
C     REAL*8 A(25,3)
      REAL KHALF,DE,KB
C
      IF(FLAG3 .EQ. 1. .AND. T .EQ. 1. .AND. IGUESS .EQ. 3)THEN
          OPEN (7,FILE='OXYGEN.OUT')
          WRITE(7,10)
10        FORMAT(' ',4X,"T",5X,"LAYER",2X,"TS(I,M)",3X,"RO2(I,2)",
    &4X,"C(I)")
      ENDIF
C
C     SURFACE OXYGEN CONCENTRATION AND LIMITING OXYGEN CONC.
      CO = 0.21/(RR*TS(1,M))
      KHALF = 0.05*CO
C
       DO 29 I=1,25
         DO 28 J=1,3
           A(I,J) = 0.0
           W(I) = 0.
28       CONTINUE
29     CONTINUE
C
C      THE FOLLOWING CALCULATIONS ARE FOR THE UNSATURATED ZONE
       DO 35 I=1,LC
C
C        THE EQUATION USED HAS A LIMITING FACTOR OF NA(I) > 0.05
         IF ( NA(I) .LE. 0.05) THEN
           XNA = 0.055
         ELSE
           XNA = NA(I)
         END IF
C
C        IF FREEZING OCCURS IN THE TOP LAYER THEN THE
C        AIR CONTENT IS SET EQUAL TO 0.1
         IF ( I .EQ. 1 .AND. TS(1,M) .LE. 273. ) THEN
           XNA = 0.1
         ENDIF
C
         DE(I) = 52.56*( ( XNA - 0.05 )/0.95 )**(1.7)
C        FOR THE UNSATURATED ZONE, RO2- (MOLES/(M3 AIR MTH)
C        FOR THE CAPILLARY FRINGE + SAT'D, RO2- (MOLES/M3 WATER MTH)
         R(I) = -RO2(I,2)
         KB(I) = R(I)/KHALF
C
         IF ( KB(I) .GT. 0.) THEN
           UR(I) = (KB(I)/DE(I))**(0.5)
         ELSE
          UR(I) = 0.
         END IF
C
         IF ( UR(I)  .GT. 0.) THEN
C
           IF ( UR(I) .GE. 60. ) THEN
             CONT2(I) = 0.
           ELSE
             CONT2(I) = 1/SINH( UR(I)*DX(I) )
           ENDIF
           IF ( UR(I) .GE. 10.) THEN
             CONT1(I) = 1.
           ELSE
             CONT1(I) = COSH( UR(I)*DX(I) )/SINH( UR(I)*DX(I) )
           ENDIF
C
         ELSE
           CONT1(I) = 0.
           CONT2(I) = 0.
         END IF
         C(I) = CO
35    CONTINUE
C
C
      DO 120  LOOP =1,5
C
        ICOUNT=0
100     CONTINUE
        ICOUNT = ICOUNT + 1
C
        DO 30 I=1,LC
C       FOLLOWING ARE CALCULATIONS FOR THE UNSATURATED ZONE
C
C     CASE I
C     UPPER BOUNDRY (IE FOR I=1)
C
      IF(I.EQ.1) THEN
C
C     CASE 1.1
C
        IF((PYR(1,3).GT.0).AND.(PYR(2,3).GT.0).AND.(C(1).GT.KHALF)
     &  .AND. (C(2).GT.KHALF)) THEN
          A(1,1)=0
          A(1,2)=-(DE(1)/DX(1)+DE(2)/DX(2))
          A(1,3)=DE(2)/DX(2)
          W(1)=R(1)*DX(1)/2.+R(2)*DX(2)/2.-DE(1)/DX(1)*CO
C
C     CASE 1.2
C
         ELSEIF((PYR(1,3).GT.0).AND.(PYR(2,3).GT.0).AND.
     &   (C(1).LE.KHALF).AND.(C(2).LE.KHALF)) THEN
          A(1,1)=0
          A(1,2)=-(UR(1)*DE(1)*CONT1(1) +
     1                   UR(2)*DE(2)*CONT1(2))
```

```
            A(1,3)=DE(2)*UR(2)*CONT2(2)
            W(1)=-DE(1)*UR(1)*CONT2(1)*CO
C
C       CASE 1.3
C
          ELSEIF((PYR(1,3).LE.0).AND.(PYR(2,3).LE.0)) THEN
            A(1,1)=0
            A(1,2)=-(DE(1)/DX(1)+DE(2)/DX(2))
            A(1,3)=DE(2)/DX(2)
            W(1)=-DE(1)/DX(1)*CO
C
C       CASE 1.4
C
          ELSEIF((PYR(1,3).LE.0).AND.(PYR(2,3).GT.0).AND.
     &    (C(2).GT.KHALF))THEN
            A(1,1)=0
            A(1,2)=-(DE(1)/DX(1)+DE(2)/DX(2))
            A(1,3)=DE(2)/DX(2)
            W(1)=R(2)*DX(2)/2-DE(1)*CO/DX(1)
C
C       CASE 1.5
C
          ELSEIF((PYR(1,3).LE.0).AND.(PYR(2,3).GT.0).AND.
     &      (C(2).LE.KHALF)) THEN
            A(1,1)=0
            A(1,2)=-(DE(1)/DX(1)+DE(2)*UR(2)*CONT1(2))
            A(1,3)=DE(2)*UR(2)*CONT2(2)
            W(1)=-DE(1)*CO/DX(1)
C
C       CASE 1.6
C
           ELSEIF((PYR(1,3).GT.0).AND.(PYR(2,3).GT.0).AND.(C(1)
     &     .GT.KHALF).AND.(C(2).LE.KHALF)) THEN
            A(1,1)=0
            A(1,2)=-(DE(1)/DX(1)+DE(2)*UR(2)*CONT1(2))
            A(1,3)=DE(2)*UR(2)*CONT2(2)
            W(1)=-R(1)*DX(1)/2.-DE(1)*CO/DX(1)
          ENDIF
C
C       CASE 2.0
C       NON-BOUNDRY UNSATURATED ZONE
C
        ELSEIF(I.LT.LC) THEN
C
C       CASE 2.1
C
        IF((PYR(I,3).GT.0).AND.(PYR(I+1,3).GT.0).AND.
     &    (C(I).GT.KHALF).AND.(C(I+1).GT.KHALF))THEN
            A(I,1)=DE(I)/DX(I)
            A(I,2)=-(DE(I)/DX(I)+DE(I+1)/DX(I+1))
            A(I,3)=DE(I+1)/DX(I+1)
            W(I)=R(I)*DX(I)/2.+R(I+1)*DX(I+1)/2.
C
C       CASE 2.2
C
```

```
         ELSEIF((PYR(I,3).GT.0).AND.(PYR(I+1,3).GT.0).AND.
     &   (C(I).LE.KHALF).AND.(C(I+1).LE.KHALF))THEN
            A(I,1)=DE(I)*UR(I)*CONT2(I)
            A(I,2)=-(UR(I)*DE(I)*CONT1(I)
     &              +UR(I+1)*DE(I+1)*CONT1(I+1))
            A(I,3)=UR(I+1)*DE(I+1)*CONT2(I+1)
            W(I)=0
C
C       CASE 2.3
C
          ELSEIF((PYR(I,3).LE.0).AND.(PYR(I+1,3).LE.0))THEN
            A(I,1)=DE(I)/DX(I)
            A(I,2)=-(DE(I)/DX(I)+DE(I+1)/DX(I+1))
            A(I,3)=DE(I+1)/DX(I+1)
            W(I)=0
C
C       CASE 2.4
C
          ELSEIF((PYR(I,3).LE.0).AND.(PYR(I+1,3).GT.0).AND.
     &     (C(I+1).GT.KHALF)) THEN
            A(I,1)=DE(I)/DX(I)
            A(I,2)=-(DE(I)/DX(I)+DE(I+1)/DX(I+1))
            A(I,3)=DE(I+1)/DX(I+1)
            W(I)=R(I+1)*DX(I+1)/2.
C
C       CASE 2.5
C
          ELSEIF((PYR(I,3).LE.0).AND.(PYR(I+1,3).GT.0).AND.
     &      (C(I+1).LE.KHALF)) THEN
            A(I,1)=DE(I)/DX(I)
            A(I,2)=-(DE(I)/DX(I)+DE(I+1)*UR(I+1)*CONT1(I+1))
            A(I,3)=DE(I+1)*UR(I+1)*CONT2(I+1)
            W(I)=0.
C
C       CASE 2.6
C
          ELSEIF((PYR(I,3).GT.0).AND.(PYR(I+1,3).GT.0).AND.(C(I).GT.
     &     KHALF).AND.(C(I+1).LE.KHALF)) THEN
            A(I,1)=DE(I)/DX(I)
            A(I,2)=-(DE(I)/DX(I)+DE(I+1)*UR(I+1)*CONT1(I+1))
            A(I,3)=DE(I+1)*UR(I+1)*CONT2(I+1)
            W(I)=R(I)*DX(I)/2.
          ENDIF
C
C       CASE 3.0
C       LOWER BOUNDRY (IE. I=LC)
C
        ELSEIF(I.EQ.LC) THEN
C
C       CASE 3.1
C
          IF((PYR(LC,3).GT.0).AND.(C(LC).GT.KHALF))THEN
            A(LC,1)=DE(LC)/DX(LC)
            A(LC,2)=-(DE(LC)/DX(LC)+INFILT(I,M)*HENRY)
            A(LC,3)=0.
```

```
              W(LC)=R(LC)/2*DX(LC)
C
C         CASE 3.2
C
            ELSEIF((PYR(LC,3).GT.0).AND.(C(LC).LE.KHALF))THEN
              A(LC,1)=DE(LC)*UR(LC)*CONT2(LC)
              A(LC,2)=-(UR(LC)*DE(LC)*CONT1(LC)
     &                      + INFILT(I,M)*HENRY)
              A(LC,3)=0.
              W(LC)=0.
C
C         CASE 3.3
C
            ELSEIF(PYR(LC,3).LE.0) THEN
              A(LC,1)=DE(LC)/DX(LC)
              A(LC,2)=-(DE(LC)/DX(LC)+INFILT(I,M)*HENRY)
              A(LC,3)=0.
              W(LC)=0.
C
            ENDIF
          ENDIF
C
30        CONTINUE
C
          CALL MATRIX(A,C,W,LC)
C
          IF(ICOUNT.EQ.3) GOTO 110
          DO 40 I=1,LC
            IF(C(I).LE.0) THEN
              DO 50 J=I,LC
 50             C(J)=0
              GOTO 100
            ENDIF
 40       CONTINUE
C
 110      CONTINUE
C
 120      CONTINUE
C
C
C         THE FOLLOWING CALCULATIONS ARE FOR THE SATURATED ZONE
C         AND THE CAPILLARY FRINGE
C
C         PLACING A LOWER LIMIT ON THE WATER OXYGEN CONC.
          IF (C(LC) .LT. 1.E-15 ) THEN
               DO 225 I=LC,LAYER
                  C(I) = 1.E-15
225            CONTINUE
          ELSE
            CW(LC) = C(LC)/HENRY
            SUMX = 0.
            XX = 0.
C
            IF (KB(LC) .LE. 0.) THEN
              KB(LC) = 0.
```

```
         ENDIF
C
         DO 130 I = LC+1,LAYER
           XX = SUMX + 0.5*DX(I)
C        NOTE THAT THE RO2 USED BELOW IS IN MOLES/(M3 WATER MTH)
C
         XY =  KB(LC)*XX/INFILT(I,M)
C
         IF ( XY  .GT. 30.) THEN
            XY = 30.
         ENDIF
         CW(I) = CW(LC)*EXP(-XY)
         SUMX = SUMX + DX(I)
C        ASSUMING A PSEUDO AIR CONCENTRATION
         C(I) = CW(I)*HENRY
C
130     CONTINUE
C
      ENDIF
C
C       THE FOLLOWING CONVERTS OXYGEN FROM MOLE/M3 TO ATM.
        DO 150 I=1,LAYER
          IF ( C(I) .LE. 1.E-20 ) THEN
             C(I) = 0.
          END IF
          COX(I,2) = C(I)
          PO2(I,2) = C(I)*RR*TS(I,M)
C
150     CONTINUE
C
         IF ( M .EQ. MONTH .AND. FLAG3 .EQ. 1. .AND. IGUESS .EQ.3)THEN
         DO 171 I = 1,LAYER
           WRITE(7,160) T,I,TS(I,M),RO2(I,2),C(I)
 160        FORMAT(' ',E10.2,1X,I3,3(1X,E10.4))
 171      CONTINUE
         ENDIF
C
        RETURN
        END
C
        SUBROUTINE MATRIX(A,C,W,LC)
        INTEGER LC
C
        INCLUDE 'MODEL.INC'
C
C       TRI DIAGONAL MATRIX SOLVER
C
C       REAL*8 A(25,3)
        REAL C(25),W(25),A(25,3)
C
C       DECOMPOSITION ROUTINE
C
        DO 250 I=2,LC
C
           IF (   A(I-1,2)  .LT. 0.) THEN
```

```
               IF ( ABS( A(I-1,2) ) .LT. 1.E-15) THEN
                    A(I-1,2) = -1.E-15
               ENDIF
           ELSE
              IF ( A(I-1,2) .LT. 1.E-15) THEN
                   A(I-1,2) = 1.E-15
              ENDIF
           ENDIF
          A(I,1)=A(I,1)/A(I-1,2)
          A(I,2)=A(I,2)-A(I,1)*A(I-1,3)
250     CONTINUE
C
C       FORWARD SUBSTITUTION
C
        DO 300 I=2,LC
C
           IF (   A(I,1)  .LT. 0.) THEN
               IF ( ABS( A(I,1) ) .LT.  1.E-15) THEN
                    A(I,1) = -1.E-15
               ENDIF
           ELSE
              IF ( A(I,1) .LT. 1.E-15) THEN
                   A(I,1) = 1.E-15
              ENDIF
           ENDIF

          W(I) = W(I) - A(I,1)*W(I-1)
C
300     CONTINUE
C
C       BACKWARD SUBSTITUTION
C
        C(LC)=W(LC)/A(LC,2)
        DO 350 K=2,LC
          I=LC-K+1
C
             C(I)=(W(I)-A(I,3)*C(I+1))/A(I,2)
350     CONTINUE
C
        RETURN
        END
```

```
      SUBROUTINE PYRITE
C
      DIMENSION K(25,3)
      REAL*4 K
      REAL*8 X5
      INCLUDE 'INTERM.INC'
      INCLUDE 'MODEL.INC'
C
C     INITIALIZING
      IF ( T .EQ. 1. ) THEN
        TOT(I,3) = 0.
      ENDIF
C
      IF (FLAG4 .EQ. 1. .AND. T .EQ. 1. .AND. I .EQ. 1.) THEN
          OPEN(8,FILE="PYRITE.OUT")
      ENDIF
      IF (FLAG4 .EQ. 1. .AND. M .EQ. MONTH .AND. IGUESS .EQ. 3 .AND.
     &I .EQ. 1.)THEN
          WRITE(8,35)
35        FORMAT(' ',4X,"T",5X,"LAYER",2X,"R1B(I,2)",3X,"R2(I,3)",3X,
     &"RT(I,2)",2X,"ALPHAP(I,2)",2X,"PYR(I,2)",2X,"PYR(I,3)")
      END IF
C
C     INITIALIZING
C
C      DETERMINING THE AVERAGE OXYGEN CONC. IN THE UNSATURATED ZONE
       IF ( I .GT. LC) THEN
         IF ( I .EQ. 1) THEN
            PI = 0.21
            DELTA = (PI + PO2(I,2))/2.0
         ELSE
            DELTA = (PO2(I-1,2)+PO2(I,2))/2.0
         ENDIF
C      OXYGEN CONC. IN THE SATURATED ZONE AND CAPILLARY FRINGE
       ELSE
          DELTA = PO2(I,2)
       ENDIF
C
       IF (DELTA .LT. 0.) THEN
           DELTA = 0.
       ENDIF
       IF (DELTA .GT. 0.21) THEN
           DELTA = 0.21
       ENDIF
C
C
C     IF THE PYRITE HAS ALREADY BEEN DEPLETED.
      IF (PYR(I,3) .LE. 1.E-10 ) THEN
        PYR(I,2) = 0.
        RAD(I,2) = 0.
        NP(I,2) = 0.
        AS(I,2) = 0.
        R2(I,2) = 0.
        R1B(I,2) = 0.
        RT(I,2) = 0.
        K(I,2) = 0.
        ALPHAP(I,2) = 0.
C
C
        IF( IGUESS .EQ. 3 )THEN
           WRITE(*,80) I
80         FORMAT(' ',"PYRITE HAS BEEN DEPLETED IN LAYER ",I2)
        ENDIF
C
        RETURN
      END IF
C
C      OVERALL REACTION RATE, RT
C
C      RECALCULATING THE CHEMICAL RATE WITH THE CURRENT O2 CONC.
C      NOTE THAT IT IS A MIXTURE OF MONOD AND FIRST ORDER KINETICS
C
       R1B(I,2)=  R1(I,2)*DELTA/(LIMO2+DELTA)
C
       R2(I,2) = -KC(I,M)*FPH*DELTA
C
       RT(I,2) = R1B(I,2)+R2(I,2)
C
C      RATE CONSTANT, K
       K(I,2) = -RT(I,2)/MOLARD
C
C      CALCULATING THE PYRITE DEPLETION
C      PYR IS THE AMOUNT OF PYRITE PER VOLUME OF TAILINGS
C
       IF ( RT(I,2) .EQ. 0.) THEN
          ALPHAP(I,2) = ALPHAP(I,3)
          PYR(I,2) = PYR(I,3)
       ELSE
         TOT(I,2) = TOT(I,3) + K(I,2)*DT
         IF (TOT(I,2) .LT. 1.E-15) THEN
             TOT(I,2) = 0.0
         END IF
C
         A1 = -COEFX*(1 - 3.*ALPHA/(ALPHA-1.) + 3.*ALPHA/(ALPHA-2.)
     &                    - ALPHA/(ALPHA-3.))
         A2 =  COEFY*(1. - 3.*BETA/(BETA-1.) + 3.*BETA/(BETA-2.)
     &                    - BETA/(BETA-3.))
         A3 = -1.*(COEFX*3.*ALPHA/(ALPHA-1.) - COEFY*3.*BETA/
     &                  (BETA-1.))
         A4 =  COEFX*3.*ALPHA/(ALPHA-2.) - COEFY*3.*BETA/(BETA-2.)
         A5 = -1.*(COEFX*ALPHA/(ALPHA-3.) - COEFY*BETA/(BETA-3.))
         X1 = A1*(TOT(I,2)/RADMAX)**ALPHA
         X2 = A2*(TOT(I,2)/RADMAX)**BETA
         X3 = A3*(TOT(I,2)/RADMAX)
         X4 = A4*(TOT(I,2)/RADMAX)**2
         X5 = A5*(TOT(I,2)/RADMAX)**3
C
         TOT(I,3) = TOT(I,2)
C
         FACT1 = (1. +X1 + X2 + X3 + X4 + X5)
```

```
C
          PYR(I,2) = PYR(I,1)*FACT1
C
C         CALCULATING SURFACE AREA PER VOLUME OF TAILINGS (M2/M3)
C
          Y1 = -1/(MOLARD*RADMAX)
          IF ( TOT(I,2) .EQ. 0. .AND. ALPHA .LT. 1.0) THEN
             Y2 = 0.
          ELSE
            Y2 = A1*ALPHA*(TOT(I,2)/RADMAX)**(ALPHA-1.)
          END IF
          Y3 = A2*BETA*(TOT(I,2)/RADMAX)**(BETA-1.)
          Y4 = A3 + 2.*A4*(TOT(I,2)/RADMAX)
          Y5 = 3.*A5*(TOT(I,2)/RADMAX)**2.0
C
          FACT2 = Y1*(Y2+Y3+Y4+Y5)
C
          ALPHAP(I,2) = PYR(I,1)*FACT2
C
        ENDIF
C
C       ESTIMATING THE MEAN RADIUS OF PYRITE PARTICLES (M)
        RAD(I,2) = RAD(I,3) - TOT(I,2)
C
C       ESTIMATING THE SURFACE AREA PER AMOUNT OF PYRITE (M2/MOL)
        SA(I,2) = 3./(MOLARD*RAD(I,2))
C
C
C       CALCULATING THE AMOUNT OF PYRITE (MOL)
        NP(I,2) = PYR(I,2)*VT(I)
C
C       CALCULATING THE PYRITE SURFACE AREA (M2)
        AS(I,2) = ALPHAP(I,2)*VT(I)
C
        IF (M .EQ. MONTH .AND. FLAG4 .EQ. 1. .AND. IGUESS .EQ.3)THEN
           WRITE(8,300) T,I,R1B(I,2),R2(I,2),RT(I,2),
     &     ALPHAP(I,2),PYR(I,2),PYR(I,3)
300        FORMAT(' ',E10.2,1X,I3,6(1X,E10.3))
        ENDIF
C
        RETURN
        END
```

```
C FILE 'SAMPLE.FOR'
C
      SUBROUTINE CREATE
C
C     THIS ROUTINE GENERATES COMPLEMENTARY CUMULATIVE PROB-
C     ABILITY FUNCTIONS (CPF) FOR INPUT ARBITRARY
C     DISTRIBUTIONS.
C
      INCLUDE 'PARAM.INC'
      INCLUDE 'COUNTS.INC'
      REAL*4 MAX,MIN,SUM
C
C     CHECK IF THERE ARE ANY ARBITRARY DISTRIBUTIONS
C
      IF (NARB.NE.0) THEN
         DO 10 I=1, NPARM
            IF (NTYPE(I).EQ.8.OR.NTYPE(I).EQ.9) THEN
               MIN=P1(I)
               MAX=P2(I)
C
C                 INITIALIZE ARBITRARY DISTRIBUTIONS
C
                  UNIT(I)=(MAX-MIN)/(FLOAT(NACELL(I))-1.)
                  ORIGIN(I)=MIN-UNIT(I)
C
C              CALCULATE CUMULATIVE PROBABILITY FUNCTIONS
C
               SUM=0.0
               DO 1800 J=1,NACELL(I)
                  SUM=SUM+V(I,J)
                  CPF(I,J)=SUM
1800           CONTINUE
               DO 1900 J=1,NACELL(I)
                  CPF(I,J)=CPF(I,J)/SUM
1900           CONTINUE
            ENDIF
 10      CONTINUE
      ENDIF
      RETURN
      END
C
C
C
      SUBROUTINE CHOOSE (I)
C
C     THIS ROUTINE WILL RETURN A VALUE FOR EACH PARAMETER.
C     IT CALLS THE APPROPRIATE SUBROUTINE DEPENDING ON THE
C     TYPE OF DISTRIBUTION SPECIFIED:
C                                         1 = CONSTANT
C                                         2 = NORMAL
C                                         3 = LOG NORMAL
C                                         4 = UNIFORM
C                                         5 = LOG UNIFORM
C                                         6 = TRIANGULAR
C                                         7 = WEIBULL
```

```
C                                           8 = BETA
C                                           9 = ARBITRARY
C                                          10 = CORRELATED
C
      INCLUDE 'INPT.INC'
      INCLUDE 'PARAM.INC'
      INCLUDE 'COUNTS.INC'
      IF (NTYPE(I).EQ.1) THEN
         XIN(I) = P1(I)
      ELSEIF (NTYPE(I).EQ.2) THEN
         CALL NORMAL (NSTART,P1(I),P2(I),P3(I),P4(I),XIN(I))
      ELSEIF (NTYPE(I).EQ.3) THEN
         CALL LNORM (NSTART,P1(I),P2(I),P3(I),P4(I),XIN(I))
      ELSEIF (NTYPE(I).EQ.4) THEN
         CALL UNIFOR (NSTART,P1(I),P2(I),XIN(I))
      ELSEIF (NTYPE(I).EQ.5) THEN
         CALL LOGUNI (NSTART,P1(I),P2(I),XIN(I))
      ELSEIF (NTYPE(I).EQ.6) THEN
         CALL TRIANG (NSTART,P1(I),P2(I),P3(I),XIN(I))
      ELSEIF (NTYPE(I).EQ.7) THEN
         CALL WEIBUL (NSTART,P1(I),P2(I),P3(I),XIN(I))
      ELSEIF (NTYPE(I).EQ.8) THEN
         CALL BETA (NSTART,P1(I),P2(I),P3(I),P4(I),XIN(I))
      ELSEIF (NTYPE(I).EQ.9) THEN
         CALL ARB (NSTART,I,XIN(I))
      ELSEIF (NTYPE(I).EQ.10) THEN
         CALL CORREL (NSTART,P1(I),P2(I),P3(I),P4(I),P5(I),CORNUM(I),
     &        XIN(I))
      ENDIF
      RETURN
      END
C
C
C
      SUBROUTINE NORMAL (NSTART,EXPECT,STDEV,MIN,MAX,XIN)
C
C     THIS ROUTINE GENERATES NORMALLY DISTRIBUTED VARIATES USING
C     THE INVERSE NORMAL CUMULATIVE PROBABILTY FUNCTION WITH n=2
C
      REAL*4 XIN,MIN,MAX,EXPECT,STDEV,R,V,T,Z,X
1000  CONTINUE
         R=RANDOM(NSTART)
         V=R-0.5
         T=SQRT(-ALOG(V*V))
         X=T-(2.30753+T*0.27061)/(1.+T*(0.99229+T*0.04481))
         Z=SIGN(X,V)
         XIN=Z*STDEV+EXPECT
      IF (XIN.LT.MIN.OR.XIN.GT.MAX) GOTO 1000
      RETURN
      END
C
C
C
      SUBROUTINE LNORM (NSTART,GM,GSD,MIN,MAX,XIN)
C
```

```
C     THIS ROUTINE GENERATES LOG-NORMALLY DISTRIBUTED VARIATES
C
      REAL*4 GM, GSD, LGM, LGSD, TMIN, TMAX, TEMP, MIN, MAX, XIN
      LGM=ALOG10(GM)
      LGSD=ALOG10(GSD)
      IF (MIN.LE.0.0) THEN
         TMIN=-1.0E37
      ELSE
         TMIN=ALOG10(MIN)
      ENDIF
      TMAX=ALOG10(MAX)
      IF (TMIN.GT.TMAX) THEN
         TEMP=TMIN
         TMIN=TMAX
         TMAX=TEMP
      ENDIF
      CALL NORMAL (NSTART,LGM,LGSD,TMIN,TMAX,TEMP)
      XIN=10.**TEMP
      RETURN
      END
C
C
C
      SUBROUTINE UNIFOR (NSTART,UMIN,UMAX,XIN)
C
C    THIS ROUTINE GENERATES UNIFORMLY DISTRIBUTED RANDOM NUMBERS
C    BETWEEN UMIN AND UMAX
C
      REAL*4 RANDOM,R,XIN,UMIN,UMAX
1000  R=RANDOM(NSTART)
      IF (UMIN.LE.UMAX) THEN
         XIN=UMIN+R*(UMAX-UMIN)
      ELSE
         XIN=UMAX+R*(UMIN-UMAX)
      ENDIF
      RETURN
      END
C
C
C
      SUBROUTINE LOGUNI (NSTART,LMIN,LMAX,XIN)
C
C    THIS ROUTINE GENERATES LOG-UNIFORMLY DISTRIBUTED RANDOM NUMBERS
C    BETWEEN LMIN AND LMAX
C
      REAL*4 RANDOM,R,XIN,LMIN,TEMP,LMAX
1000  R=RANDOM(NSTART)
      TEMP=ALOG10(LMIN)+R*(ALOG10(LMAX)-ALOG10(LMIN))
      XIN=10**TEMP
      RETURN
      END
C
C
C
      SUBROUTINE TRIANG (NSTART,VMIN,VMODE,VMAX,XIN)
```

```
C
C       THIS ROUTINE GENERATES TRIANGULARLY DISTRIBUTED VARIATES
C
      REAL*4 XIN,R,VMAX,VMIN,VMODE,Z1,Z2
1000  R=RANDOM(NSTART)
      Z1=VMAX-VMIN
      Z2=VMODE-VMIN
      IF (R.LE.Z2/Z1) THEN
         XIN=VMIN+SQRT(R*Z1*Z2)
      ELSE
         XIN=VMAX-SQRT((1.-R)*(VMAX-VMODE)*Z1)
      ENDIF
      RETURN
      END
C
C
C
      SUBROUTINE WEIBUL (NSTART,A,B,C,XIN)
C
C     THIS SUBROUTINE GENERATES RANDOM SAMPLES FROM WEIBULL
C     DISTRIBUTIONS BY TRANSFORMING UNIFORMLY DISTRIBUTED SAMPLES
C     TO A SPECIFIED WEIBULL DISTRIBUTION
C
      REAL*4 A,B,C,XIN,R
      INTEGER*4 NSTART
1000  R=RANDOM(NSTART)
      XIN=A+B*((-ALOG(R))**(1.0/C))
      RETURN
      END
C
C
C
      SUBROUTINE BETA (NSTART,MIN,MAX,A,B,XIN)
C
C     THIS SUBROUTINE GENERATES BETA DISTRIBUTED RANDOM NUMBERS USING
C     THE ACCEPTANCE-REJECTION METHOD A IF a OR b < or = 1 AND
C     METHOD B IF a OR b >1.
C
      REAL*4 MIN,MAX,A,B,XIN,R1,R2,V1,V2,W,AM1,BM1,ABM2,TEMP
      IF (A.LE.1.0.OR.B.LE.1.0) THEN
C
C        USE ACCEPTANCE-REJECTION METHOD A
C
10       CONTINUE
11          CONTINUE
               R1=RANDOM(NSTART)
               R2=RANDOM(NSTART)
               V1=R1**(1/A)
               V2=R2**(1/B)
               W=V1+V2
               IF (W-1.0) 20,20,11
20          CONTINUE
            XIN=V1/W
         IF (XIN.LT.MIN.OR.XIN.GT.MAX) GOTO 10
      ELSE
```

```
C
C     USE ACCEPTANCE-REJECTION METHOD B
C
         AM1=A-1.
         BM1=B-1.
         ABM2=AM1+BM1
         F=(ABM2**ABM2)/((AM1**AM1)*(BM1**BM1))
110      CONTINUE
111         CONTINUE
               R1=RANDOM(NSTART)
               R2=RANDOM(NSTART)
               XIN=R1
               TEMP=(XIN**AM1)*((1.-XIN)**BM1)*F
               IF (R2-TEMP) 120,111,111
120         CONTINUE
         IF (XIN.LT.MIN.OR.XIN.GT.MAX) GOTO 110
      ENDIF
      RETURN
      END
C
C
C
      SUBROUTINE ARB (NSTART,I,XIN)
C
C      THIS ROUTINE SAMPLES VALUES OF ARBITRARY VARIATES.
C
      INCLUDE 'PARAM.INC'
      INTEGER*2 ICELL,I
      REAL*4 XIN,R
      R=RANDOM(NSTART)
      DO 1100 ICELL=1,NACELL(I)
         IF (CPF(I,ICELL).GE.R) GOTO 1000
1100  CONTINUE
      ICELL=NACELL(I)
1000  XIN=ORIGIN(I)+ICELL*UNIT(I)
      RETURN
      END
C
C
C
      SUBROUTINE CORREL(NSTART,MEANY,SDEVY,CCOEFF,MEANX,SDEVX,CORNUM,XIN
     &)
C
C     THIS SUBROUTINE CALCULATES THE VALUE OF AN INPUT PARAMETER WHICH
C     IS CORRELATED WITH SOME PREVIOUS INPUT PARAMETER.  IT EMPLOYS
C     KLEIJNEN'S CORRELATED GENERATION TECHNIQUE (KLEIJNEN, J.P.C.
C     (1974) STATISTICAL TECHNIQUES IN SIMULATION - PART 1, MARCEL
C     DEKKER,N.Y.) AS PRESENTED BY ANDRES AND GOODWIN (1984).
C
      INCLUDE 'INPT2.INC'
      INTEGER*2 CORNUM
      REAL*4 MEANY,SDEVY,CCOEFF,MEANX,SDEVX,XIN,A,B,U,Z,X,Y
      A=CCOEFF*SDEVY/SDEVX
      B=MEANY-CCOEFF*MEANX*SDEVY/SDEVX
      CALL NORMAL (NSTART,0.0,1.0,-1.0E37,1.0E37,Z)
      U=SDEVY*Z*SQRT(1.0-CCOEFF**2)
      X=XVALUE(CORNUM)
      Y=A*X+B+U
      XIN=Y
      RETURN
      END
C
C
C
      FUNCTION RANDOM (NSTART)
C
C     THIS PORTABLE FORTRAN RANDOM NUMBER GENERATOR WAS
C     ADAPTED FROM THAT DESCRIBED BY K. MARSE AND S.D. ROBERTS
C     ('SIMULATION', OCTOBER, 1983; PP 135-139)
C
      INTEGER*4 B2E15,B2E16,H115,H131,LOW15,LOWPRD,MODLUS,
     &          MULT1,MULT2,OVFLOW
      MULT1=24112
      MULT2=26143
      B2E15=32768
      B2E16=65536
      MODLUS=2147483647
      H115=NSTART/B2E16
      LOWPRD=(NSTART-H115*B2E16)*MULT1
      LOW15=LOWPRD/B2E16
      H131=H115*MULT1+LOW15
      OVFLOW=H131/B2E15
      NSTART=(((LOWPRD-LOW15*B2E16)-MODLUS)+
     &   (H131-OVFLOW*B2E15)*B2E16)+OVFLOW
      IF (NSTART.LT.0) NSTART=NSTART+MODLUS
      H115=NSTART/B2E16
      LOWPRD=(NSTART-H115*B2E16)*MULT2
      LOW15=LOWPRD/B2E16
      H131=H115*MULT2+LOW15
      OVFLOW=H131/B2E15
      NSTART=(((LOWPRD-LOW15*B2E16)-MODLUS)+(H131-OVFLOW*B2E15)*B2E16)
     &   +OVFLOW
      IF (NSTART.LT.0) NSTART=NSTART+MODLUS
      RANDOM=(2*(NSTART/256)+1)/16777216.0
      RETURN
      END
      SUBROUTINE SPECIATION
C
C
C
      INCLUDE 'INTERM.INC'
      INCLUDE 'MODEL.INC'
C
      REAL HCO31,HCO32,HI,TRIP,TOLER,FN1,FN2,PH1,PH2,SUM
      DIMENSION X1(300)
      INTEGER NPHIT
      IF (IGUESS .EQ. 3 .AND.FLAG6 .EQ. 1. .AND. T .EQ. 1. .AND.
     &I .EQ. 1.) THEN
           OPEN(10,FILE="SPECIATI.OUT")
           WRITE(10,15)
15         FORMAT(' ',4X,"T",7X,"I",2X,"CASE(I)",2X,"PH(I,2)",3X,
     &"PH(I,3)",2X,"NPHIT")
      ENDIF
C
C
C      BOTH CALCITE AND GYPSEM PRESENT
C        (ANALYTICAL SOLUTIONS)
C
      IF ( CASE(I) .EQ. 'C111') THEN
C
        NPHIT = 1
C
C       OPEN SYSTEM
C
C       NOTE KCO2 IS IN UNITS OF MOL/L.ATM
C
          HI = (DK1*DK2*KCO2*PCO2(I,2)*F(2)*
     &         CA(I,2)/KCACO3)**0.5
          CT(I,2) = PCO2(I,2)*KCO2*((HI+DK1)/HI)
C
C
          HCO3(I,2) = (DK1/(HI+DK1))*CT(I,2)
          PH(I,2) = -ALOG10(HI)
          DELCAL(I) = DELCAL(I)
C
          GOTO 600
C
      ELSE  IF (CASE(I) .EQ. 'C112') THEN
C
C       CLOSED SYSTEM
C
          FE2(I,2)  = FE2T(I,2)
          CT(I,2) = CTT(I,2)
          IF (I .GE. LC .AND. CACO3(I,3) .GT. 0.) THEN
              CT(I,2) = SATCT
          ENDIF
          BBB = POTAS(I,2)/2. + FE2T(I,2) -
     &         (CT(I,2)/2.)*DK1/(DK1+10**(-PH(I,3)))
          CONST = (KCASO4/F(2)**2.)*(1.+CHSO4*
     &             10**(-PH(I,3))*F(2)/F(1))
          CA(I,2) = (-BBB+(BBB**2. + 4*CONST)**(0.5) )/2.
          S04(I,2) = CONST/CA(I,2)
          HC03(I,2) = 2*CA(I,2)+POTAS(I,2) + 2*FE2(I,2) -2*S04(I,2)
          HI = HC03(I,2)*DK2*CA(I,2)*F(1)*F(2)/KCAC03
          PH(I,2) = -ALOG10(HI)
          DELCAL(I) = DELCAL(I)
C
          GOTO 600
C
      ELSE
C         CALCITE OR GYPSUM IS ABSENT
          DELCAL(I) = 0.0
      ENDIF
C
C     REMAINING SOLUTIONS ARE ITERATIVE
C
C     IN THE FOLLOWING CALCULATIONS THE ROOT OF AN EQUATION
C     IS SOLVED BY BRUTE FORCE METHOD.
C
C

      IMAX = 300
      NPHIT = 0
      TOLER = 0.01
C
C     FOR THE TRIALS XI WILL REPRESENT THE "PH"
C
C     ADJUSTING THE PH SO THAT IT DOES NOT OVERSHOOT
C
      IF (PH(I,3) .LE. 0.) THEN
         PH(I,3) = 0.5
      ENDIF
      IF (CAC03(I,3) .LE. 0. .AND. ALOH3(I,3) .GT. 0. ) THEN
         IF (PH(I,3) .LE. 2.27 ) THEN
             PH(I,3) = 2.3
         ENDIF
      ENDIF
C
      XI = PH(I,3)
      X1(1) = PH(I,3)
C
      DO 200 NPHIT= 1,IMAX
C       IMAX ARE THE MAXIMUM NUMBER OF ITERATIONS ALLOWED
C
C     GENERAL VARIABLES  ( FUNCTION OF PH )
C
C     OPEN SYSTEM CASE '111'
C       PC02 IS IN ATM   , KC02 IS IN MOL/L.ATM
        HC031 = DK1*PC02(I,2)*KC02*10**XI/F(1)
        BICARBP1 = 2.303*DK1*PC02(I,2)*KC02*10**XI/F(1)
C
C     CLOSED SYSTEM CASE '112'
        CT(I,2) = CT(II,3)*FRAC*VRAIN(II,M)/VRAIN(I,M)
        HC032 = (DK1*CT(I,2))/(10**(-XI)*F(1) +DK1)
        BICARBP2 = 2.303*DK1*CT(I,2)*10**(-XI)/(10**(-XI)*F(1)
     &              +DK1)**2.
C
```

```
C
C     GYPSUM ABSENT, BUT CALCITE IS PRESENT
      IF (CASE(I) .EQ. 'C113' .OR. CASE(I) .EQ. 'C114') THEN
C
C       GENERAL VARIABLES
C
C
C      IGNORING THE CONTRIBUTION OF FE3 AND ALT
       SFACT = ( 1.+(10**(-XI)*F(2))/(F(1)*CHSO4)+CALSO4*F(3)*
     &       F(2)/F(1)*AL3(I,2)+CFESO4*F(3)*F(2)/F(1)*
     &             FE3(I,2) + CCASO4*F(2)**2.*CA(I,2)  )
       SULF(I,2) = (2+10**(-XI)*F(2)/(CHSO4*F(1)))*SO4(I,2)
C
C
        IF (CASE(I) .EQ. 'C113') THEN
C
C         OPEN SYSTEM CASE '113'
C
          CALL FNN(XI,FN)
C
        ELSE
C        CLOSED SYSTEM CASE '114'
         IF (I .GE. LC .AND. CACO3(I,3) .GT. 0.) THEN
              CT(I,2) = SATCT
         ENDIF
C
         CALL FNN(XI,FN)
C
       ENDIF
C
C     CASE 2.  BOTH FE(OH)3 AND AL(OH)3) ARE PRESENT
      ELSE  IF  (CASE(I) .EQ. 'C210' .OR. CASE(I) .EQ. 'C220') THEN
C         GENERAL VARIABLES
C
          IF (CASE(I) .EQ. 'C210') THEN
C            OPEN SYSTEM CASE '210'
             HCO3(I,2) = HCO31
             BICARBP(I,2) = BICARBP1
C
            CALL FNN(XI,FN)
C
          ELSE
C           CLOSED SYSTEM CASE '220'
            HCO3(I,2) = HCO32
            BICARBP(I,2) = BICARBP2
C
            CALL FNN(XI,FN)
C
          ENDIF
C
C     CASE 3  BOTH FE(OH)3 AND AL(OH)3 ARE ABSENT
      ELSE IF (CASE(I) .EQ. 'C310' .OR. CASE(I) .EQ. 'C320') THEN
C
          IF (CASE(I) .EQ. 'C310') THEN
C           OPEN SYSTEM CASE '310'
            HCO3(I,2) = HCO31
            BICARBP(I,2) = BICARBP1
            CALL FNN(XI,FN)
C
          ELSE
C           CLOSED SYSTEM CASE '320'
            HCO3(I,2) = HCO32
            BICARBP(I,2) = BICARBP2
           CALL FNN(XI,FN)
C
          ENDIF
C
C      CASE 4.  FE(OH)3 IS PRESENT BUT AL(OH)3 IS ABSENT
       ELSE IF (CASE(I) .EQ. 'C410' .OR. CASE(I) .EQ. 'C420') THEN
C
          IF (CASE(I) .EQ. 'C410') THEN
C           OPEN SYSTEM CASE '410'
            HCO3(I,2) = HCO31
            BICARBP(I,2) = BICARBP1
C
            CALL FNN(XI,FN)
C
          ELSE
C           CLOSED SYSTEM CASE '420'
            HCO3(I,2) = HCO32
            BICARBP(I,2) = BICARBP2
C
            CALL FNN(XI,FN)
C
          ENDIF
C
C      CASE 5.  AL(OH)3 IS PRESENT BUT FE(OH)3 IS ABSENT
       ELSE
C
          IF (CASE(I) .EQ. 'C510') THEN
C           OPEN SYSTEM CASE '510'
            HCO3(I,2) = HCO31
            BICARBP(I,2) = BICARBP1
C
            CALL FNN(XI,FN)
C
          ELSE
C           CLOSED SYSTEM CASE '520'
            HCO3(I,2) = HCO32
            BICARBP(I,2) = BICARBP2
C
            CALL FNN(XI,FN)
C
          ENDIF
C
       ENDIF
C
C
C      RE-EVALUATING THE PH VALUE
C
C      UPDATING CA AND SO4
```

```
C
      IF (XI .LT. 4.0) THEN
C
C       GYPSUM PRECIPITATION/DISSOLUTION
C
C
        SSFACT = 1.+CFESO4*F(3)*F(2)/F(1)*FE3(I,2)
     &               +CALSO4*F(3)*F(2)/F(1)*AL3(I,2)
     &               +10**(-XI)*F(2)/(CHSO4*F(1))
        A = SO4T(I,2) - CAT(I,2)
        B = KCASO4/F(2)**2*SSFACT
        CAEQU = (-A+(A**2+4*B)**(0.5))/2.
        SO4EQ = KCASO4/(F(2)**2*CAEQU)
        CA(I,2) = CAT(I,2)/(1.+CCASO4*F(2)**2*SO4(I,2) )
        IF (CAEQU .GT. CA(I,2)  .AND. GYP(I,3) .LE. 0.) THEN
           CAEQU = CA(I,2)
           SO4EQ = SO4T(I,2)/(SSFACT+CCASO4*F(2)**2*CA(I,2) )
        ENDIF
        SO4T(I,2) = SO4EQ*(SSFACT+CCASO4*F(2)**2*CAEQU)
        CATN = CAEQU*(1.+CCASO4*F(2)**2*SO4EQ)
        SO4(I,2) = SO4EQ
        CA(I,2) = CAEQU
        DGYP(I,2) = CALIN - CATN
        CAT(I,2) = CATN
C
      ENDIF
C
      IF(NPHIT .EQ. 1) THEN
        FN1 = FN
        PH1 = XI
        X1(NPHIT+1) = X1(NPHIT) + 0.10
        IF(FN1 .LT. 0.)THEN
          X1(NPHIT+1) = X1(NPHIT) - 1.0
        ENDIF
        XI = X1(NPHIT+1)
        TRIP = 0.
      ELSE
        FN2 = FN
        PH2 = XI
C
        IF(ABS(FN2) .GT. ABS(FN1) .AND. NPHIT .GT.2)THEN
          PH(I,2) = X1(NPHIT-1)
          GOTO 600
        ENDIF
C
        SUM = PH1 + PH2
        TRAP = FN1 - FN2
        TRIP = PH1 - PH2
C
        IF(ABS(TRIP) .GT. TOLER) THEN
          X1(NPHIT+1) = PH2 - FN2*(PH1-PH2)/(FN1-FN2)
C
          IF(ABS(TRAP) .LT. 0.1) THEN
            PH(I,2) = X1(NPHIT)
            GOTO 600
          ENDIF
C
          IF(FN2 .LT. 0.) THEN
            X1(NPHIT+1) = X1(NPHIT) - 0.1
          ENDIF
C
          IF(X1(NPHIT+1) .GT. 8.0) THEN
            X1(NPHIT+1) = SUM/2.
          ENDIF
C
         IF(X1(NPHIT+1)  .LT. 0.0) THEN
            X1(NPHIT+1) = SUM/2.
         ENDIF
C
          XI = X1(NPHIT+1)
          PH1 = PH2
          FN1 = FN2
        ELSE
          PH(I,2) = X1(NPHIT)
          GOTO 600
        ENDIF
      ENDIF
      IF ( NPHIT.EQ. IMAX) THEN
         CALL ERROR (53,0)
      ENDIF
C
200   CONTINUE
600   CONTINUE
C
      IF (M .EQ. MONTH .AND. FLAG6 .EQ. 1. .AND. IGUESS .EQ. 3) THEN
        WRITE(10,700) T,I,CASE(I),PH(I,2),PH(I,3),NPHIT
700     FORMAT(' ',E10.4,1X,I3,2X,A4,2X,2(E10.4,1X),I3)
      ENDIF
C
      RETURN
      END


      SUBROUTINE FNN(XI,FN)
C
      INCLUDE 'INTERM.INC'
      INCLUDE 'MODEL.INC'
C
C
C
       IF (CASE(I) .EQ. 'C210'.OR. CASE(I) .EQ. 'C220' .OR. CASE(I) .EQ.
     &    'C510' .OR. CASE(I) .EQ. 'C520') THEN
C        ALOH3 IS PRESENT
C
         XZ = KBAS-(10.*XI)
         IF ( XZ  .LT. -35.) THEN
              XZ = -35.
         ENDIF
C
         AL3(I,2) =(10**(XZ)/(SO4(I,2)*F(2)))**(0.25)/F(3)
         ALFACT = (1.+CALOH*F(3)/F(2)*10**XI+
     &            CALOH2*F(3)/F(1)*10**(2.*XI)+
     &            CALOH3*F(3)*10**(3.*XI)+
     &            CALSO4*F(3)*F(2)/F(1)*SO4(I,2))
         ALT(I,2) = ALFACT*AL3(I,2)
       ELSE
C        ALOH3 IS ABSENT
C
         ALFACT = (1.+CALOH*F(3)/F(2)*10**XI+
     &            CALOH2*F(3)/F(1)*10**(2.*XI)+
     &            CALOH3*F(3)*10**(3.*XI)+
     &            CALSO4*F(3)*F(2)/F(1)*SO4(I,2))
         AL3(I,2) = ALT(I,2)/ALFACT
       ENDIF
C
C
       IF (CASE(I) .EQ. 'C210' .OR. CASE(I) .EQ. 'C220'.OR. CASE(I) .EQ.
     &    'C410'.OR. CASE(I) .EQ. 'C420') THEN
C        FEOH3 IS PRESENT
C
         FE3SOL = KFEOOH/F(3)*10**(-3.*XI)
         FE3(I,2) = FE3SOL
         FEFACT = (1.+CFEOH*F(3)/F(2)*10**XI +
     &            CFEOH2*F(3)/F(1)*10**(2.*XI) +
     &            CFEOH3*F(3)*10**(3.*XI)+
     &            CFESO4*F(3)*F(2)/F(1)*SO4(I,2))
         FE3T(I,2) = FEFACT*FE3(I,2)
C
       ELSE
C        FEOH3 IS ABSENT
C
         FEFACT = (1.+CFEOH*F(3)/F(2)*10**XI +
     &            CFEOH2*F(3)/F(1)*10**(2.*XI) +
     &            CFEOH3*F(3)*10**(3.*XI)+
     &            CFESO4*F(3)*F(2)/F(1)*SO4(I,2))
         FE3(I,2) = FE3T(I,2)/FEFACT
C
      ENDIF
C
C
      SFACT = ( 1.+(10**(-XI)*F(2))/(F(1)*CHSO4)+
     &        CALSO4*F(3)*F(2)/F(1)*AL3(I,2)+
     &        CFESO4*F(3)*F(2)/F(1)*FE3(I,2)
     &        + CCASO4*F(2)**2.*CA(I,2)      )
C
C
      FEITY = ( 3.+2.*CFEOH*F(3)/F(2)*10**(XI)+
     &        CFEOH2/F(1)*F(3)*10**(2*XI)+
     &        CFESO4*F(3)*F(2)/F(1)*SO4(I,2))
      ALITY = ( 3.+2.*CALOH*F(3)/F(2)*10**XI +
     &        CALOH2/F(1)*F(3)*10**(2*XI)+
     &        CALSO4*F(3)*F(2)/F(1)*SO4(I,2))
      ALUM(I,2) = ALITY*AL3(I,2)
      IRON(I,2) = FEITY*FE3(I,2)
C
```

```
      SULF(I,2) = (2.+10**(-XI)*F(2)/(CHSO4*F(1)))*SO4T(I,2)/SFACT
C
C     UPDATING POTAS FOR PH CHANGE WHEN ALOH3 IS ABSENT
      IF (ALOH3(I,3) .LE. 0.) THEN
        RSER(I) = 1.6E-3*(1.-0.11*XI)
        IF (RSER(I)  .LT. 0.) THEN
            RSER(I) = 0.
        ENDIF
        POTAS(I,2) = VRAIN(II,M)*FRAC*POTAS(II,3)/VRAIN(I,M) +
     &              RSER(I)*VT(I)/VRAIN(I,M)
      ENDIF
C
      FN = 1000*( 10**(-XI)+2*CA(I,2)+ALUM(I,2)+IRON(I,2)+2*FE2T(I,2)-
     &     HCO3(I,2)-SULF(I,2)+POTAS(I,2)-NO3T(I,2) )
C
C     GYPSUM ABSENT, BUT CALCITE IS PRESENT
      IF (CASE(I) .EQ. 'C113' .OR. CASE(I) .EQ. 'C114') THEN
C
        IF (CASE(I) .EQ. 'C113') THEN
C
C         OPEN SYSTEM CASE '113'
C
          FN = 2*10**(-2.*XI)*KCACO3/(DK1*DK2*KCO2*PCO2(I,2)) +
     &       2*FE2T(I,2)+POTAS(I,2)-DK1*KCO2*PCO2(I,2)*
     &       10**XI-SULF(I,2)
C
        ELSE
C        CLOSED SYSTEM CASE '114'
C
         FN = 2*KCACO3*10**(-XI)*(10**(-XI)+DK1)/(DK1*DK2*
     &      CT(I,2)) + 2*FE2T(I,2)+POTAS(I,2)-DK1/
     &      (10**(-XI)+DK1)*CT(I,2)-SULF(I,2)
C
        ENDIF
       ENDIF
C
      RETURN
      END
```

```
C FILE 'SAVE.FOR'
C
      SUBROUTINE TIMSEL
C
C     THIS SUBROUTINE SAVES TIME-VARIANT INPUT VARIABLES
C     FLAGGED FOR OUTPUT
C
      INCLUDE 'COUNTS.INC'
      INCLUDE 'INPT.INC'
      INCLUDE 'OUT.INC'
      NUMF=1
C
C     CHECK IF ANY DISTRIBUTIONS ARE TIME-VARIANT
C
      IF (VARYF.NE.0) THEN
C
C        INITIALIZE OR INCREMENT TIME COUNTERS
C
         IF (NEWNT.EQ.0) THEN
            TNUMBF=1
            TMOBF=1
         ENDIF
C
C        CHECK IF THIS TIME TO BE SAVED
C
         NCHECK=MOD(INT(T),12)
         IF(NCHECK.EQ.0)NCHECK=12
         IF (TFILE(TMOBF).EQ.NCHECK) THEN
            DO 40 I=1,VARY
               J=VARIED(I)
C
C              CHECK IF VALUE TO BE OUTPUT
C
               IF (EFLAG(J).EQ.'F'.AND.NSTEPF.GE.TMOBF) THEN
C
C                 SORT VALUES AND SAVE
C
                  JF=NSTEPF*NYR*(NUMF-1)+NFILE+TNUMBF
                  NUMF=NUMF+1
                  XOUT(JF)=XIN(J)
               ENDIF
40          CONTINUE
            TNUMBF=TNUMBF+1
            TMOBF=TMOBF+1
            IF(TMOBF.GT.NSTEPF)TMOBF=1
         ENDIF
      ENDIF
      RETURN
      END
C
C
C
      SUBROUTINE SELECT
C
C     THIS SUBROUTINE CHECKS WHETHER PARAMETER VALUES ARE TO
```

```
C     BE SAVED AT EACH TIME, T. IT INDICATES WHETHER VALUES ARE
C     TO BE WRITTEN TO STATISTICS FILE OR DETAILED RESULTS FILE
C     VECTORS
C
      INCLUDE 'COUNTS.INC'
      NUMF=1
      NCHECK=MOD(INT(T),12)
      IF (NEWNT.EQ.0) THEN
         TNUMF=1
         TMOF=1
      ENDIF
C
C     CHECK IF THIS TIME STEP IS TO BE SAVED
C
         IF (TFILE(TMOF).EQ.NCHECK) THEN
            CALL SORT
            TNUMF=TNUMF+1
            TMOF=TMOF+1
         ENDIF
         IF(TMOF.GT.NSTEPF)TMOF=1
      RETURN
      END
C
C
C
      SUBROUTINE SORT
C
C     THIS SUBROUTINE CHECKS ALL OUTPUT ARRAYS.  FOR ANY ARRAYS
C     CONTAINING PARAMETERS TO BE SAVED, THE CURRENT PARAMETER
C     VALUE IS WRITTEN TO A DUMMY VARIABLE FOR TRANSFER TO
C     SUBROUTINE 'SEND'.
C
      INCLUDE 'COUNTS.INC'
      INCLUDE 'INFO.INC'
      INCLUDE 'INTERM.INC'
      REAL*4 XDUM
      K=1
      DO 1000 I=1,NARRAY
         IF (NVAR(I).NE.0) THEN
            DO 2000 J=1,NVAR(I)
C
C              FIND CORRECT OUTPUT VALUE
C
               IF (I.EQ.1) THEN
                  XDUM=PH(LOC(K),2)
               ELSEIF (I.EQ.2) THEN
                  XDUM=PO2(LOC(K),2)
               ELSEIF (I.EQ.3) THEN
                  XDUM=R1B(LOC(K),2)
               ELSEIF (I.EQ.4) THEN
                  XDUM=R2(LOC(K),2)
               ELSEIF (I.EQ.5) THEN
                  XDUM=RPYR(LOC(K))
               ELSEIF (I.EQ.6) THEN
                  XDUM=PYR(LOC(K),2)
                  ELSEIF (I.EQ.7) THEN
                     XDUM=FE3(LOC(K),2)
                  ELSEIF (I.EQ.8) THEN
                     XDUM=AL3(LOC(K),2)
                  ELSEIF (I.EQ.9) THEN
                     XDUM=FE2(LOC(K),2)
                  ELSEIF (I.EQ.10) THEN
                     XDUM=CA(LOC(K),2)
                  ELSEIF (I.EQ.11) THEN
                     XDUM=FE3T(LOC(K),2)
                  ELSEIF (I.EQ.12) THEN
                     XDUM=SO4T(LOC(K),2)
                  ELSEIF (I.EQ.13) THEN
                     XDUM=FE2T(LOC(K),2)
                  ELSEIF (I.EQ.14) THEN
                     XDUM=CAT(LOC(K),2)
                  ELSEIF (I.EQ.15) THEN
                     XDUM=SO4(LOC(K),2)
                  ELSEIF (I.EQ.16) THEN
                     XDUM=ALT(LOC(K),2)
                  ELSEIF (I.EQ.17) THEN
                     XDUM=AFLUX(LOC(K),2)
                  ELSEIF (I.EQ.18) THEN
                     XDUM=ATOTAL(LOC(K),2)
                  ELSEIF (I.EQ.19) THEN
                     XDUM=AYEAR(LOC(K),2)
                  ELSEIF (I.EQ.20) THEN
                     XDUM=BLANK1(LOC(K),2)
                  ELSEIF (I.EQ.21) THEN
                     XDUM=BLANK2(LOC(K),2)
                  ELSEIF (I.EQ.22) THEN
                     XDUM=BLANK3(LOC(K),2)
                  ELSEIF (I.EQ.23) THEN
                     XDUM=BLANK4(LOC(K),2)
                  ELSEIF (I.EQ.24) THEN
                     XDUM=BLANK5(LOC(K),2)
                  ENDIF
                  CALL SEND (XDUM)
                  K=K+1
2000           CONTINUE
            ENDIF
1000  CONTINUE
      RETURN
      END
C
C
C
      SUBROUTINE SEND (XDUM)
C
C     SUBROUTINE ACCEPTS THE CURRENT VALUE OF A VARIABLE AND ALLOCATES
C     IF TO AN APPROPRIATE POSITION IN THE OUTPUT VECTOR.
C
      INCLUDE 'COUNTS.INC'
      INCLUDE 'OUT.INC'
      REAL*4 XDUM
```

```
C
C     SORT OUTPUTS AND SEND THE VARIABLES TO OUTPUT VECTOR
C
      JF=(NUMF-1+VARYF)*NSTEPF*NYR+TNUMF+NFILE
      XOUT(JF)=XDUM
      NUMF=NUMF+1
      RETURN
      END
C
C
C
      SUBROUTINE SAVEIN
C
C     THIS SUBROUTINE SAVES ALL VALUES OF SELECTED NON-TIME-VARIANT
C     INPUT PARAMETERS TO VECTOR XOUT.
C
      INCLUDE 'OUT.INC'
      INCLUDE 'INPT.INC'
      INCLUDE 'COUNTS.INC'
C
C     CHECK IF ANY INPUT VALUES TO BE SAVED
C
      IF (NFILE.NE.0) THEN
         NFIL=0
         DO 10 J=1,VARN
            I=VARNOT(J)
            IF (EFLAG(I).EQ.'F') THEN
C
C              SAVE VALUE TO OUTPUT VECTOR
C
               NFIL=NFIL+1
               XOUT(NFIL)=XIN(I)
            ENDIF
10       CONTINUE
      ENDIF
      RETURN
      END
```

```
C FILE 'STATS.FOR'
C
      SUBROUTINE STATS
C
C     SUBROUTINE STATS CALCULATES SUMMARY STATISTICS FOR VARIABLES
C     CONTAINED IN THE VECTOR XOUT. THE ANALYSIS INVOLVES UPDATING
C     CALCULATIONS WHICH ARE PERFORMED IN SUBROUTINES MOMENT AND
C     GMOMENT.
C
      INCLUDE 'STATS.INC'
      INCLUDE 'OUT.INC'
      INCLUDE 'COUNTS.INC'
      INCLUDE 'UPDATE.INC'
      DOUBLE PRECISION XN,GSD(750),Z1
C
C     INITIALIZE STATISTICS ON FIRST TRIAL
C
      IF (NUMTRL.EQ.1) THEN
         NOUT=NSTEPF*(VARYF+NVARYF)*NYR+NFILE
         DO 1100 IDIST1=1,NOUT
            XMAX(IDIST1)=-1.0E+37
            XMIN(IDIST1)=+1.0E+37
            GN(IDIST1)=0
            N(IDIST1)=0
1100     CONTINUE
      ENDIF
C
C     ON EACH TRIAL, MAXIMUM,MINIMUM AND VARIOUS MOMENTS ARE UPDATED
C     FOR EACH PARAMETER.
C
      DO 1360 ID=1,NOUT
         Z1=XOUT(ID)
         IF (Z1.GT.XMAX(ID)) XMAX(ID)=SNGL(Z1)
         IF (Z1.LT.XMIN(ID)) XMIN(ID)=SNGL(Z1)
         CALL MOMENT (Z1,N(ID),S1(ID),S2(ID),S3(ID),S4(ID))
         CALL GMOMEN (Z1,GN(ID),GS1(ID),GS2(ID))
1360  CONTINUE
C
C     FOLLOWING THE FINAL TRIAL, THE CUMULATIVE MOMENT RESULTS ARE
C     USED TO CALCULATE SUMMARY STATISTICS.
C
      IF (NUMTRL.EQ.NTRIAL) THEN
         DO 1400 I=1,NOUT
            XN=DBLE(N(I))
            SDEV(I)=-999.
            SKEW(I)=-999.
            KURT(I)=-999.
            IF(N(I).GT.1)THEN
               SDEV(I)=DSQRT(S2(I)/(XN-1.0))
               IF(N(I).GT.2.AND.S2(I).GT.0.0)THEN
                  SKEW(I)=(S3(I)/XN)/((S2(I)/XN)**1.5)
                  IF(N(I).GT.3)KURT(I)=(S4(I)/XN)/((S2(I)/XN)**2.0)
               ENDIF
            ENDIF
         GMEAN(I)=-999.
```

```
            GSDEV(I)=-999.
            IF(GN(I).GE.1)THEN
               GMEAN(I)=DEXP(GS1(I))
               IF(GN(I).GE.2)THEN
                  GSD(I)=DSQRT(GS2(I)/DBLE(GN(I)-1))
                  GSDEV(I)=DEXP(GSD(I))
               ENDIF
            ENDIF
1400        CONTINUE
         ENDIF
         RETURN
         END
C
C
C
         SUBROUTINE MOMENT (X,N,S1,S2,S3,S4)
C
C        THIS SUBROUTINE CALCULATES THE FIRST FOUR MOMENTS
C        OF A RANDOM VARIABLE USING AN ALGORITHM BY C.C. SPICER
C        (APPLIED STATISTICS 21,226-227 (1972)).
C
         DOUBLE PRECISION X,S1,S2,S3,S4,AN,AN1,DX,DX2
         INTEGER*2 N
         N=N+1
         IF (N.EQ.1) THEN
            S1=X
            S2=0.0
            S3=0.0
            S4=0.0
         ELSE
            AN=N
            AN1=AN-1.0
            DX=(X-S1)/AN
            DX2=DX*DX
            S4=S4-DX*(4.0*S3-DX*(6.0*S2+AN1*(1.0+AN1**3)*DX2))
            S3=S3-DX*(3.0*S2-AN*AN1*(AN-2.0)*DX2)
            S2=S2+AN*AN1*DX2
            S1=S1+DX
         ENDIF
         RETURN
         END
C
C
C
         SUBROUTINE GMOMEN (X,N,GS1,GS2)
C
C        THIS SUBROUTINE CALCULATES THE GEOMETRIC MEAN AND
C        STANDARD DEVIATION USING THE METHOD OUTLINED IN
C        SUBROUTINE 'MOMENTS'.
C
         DOUBLE PRECISION X,GX,GS1,GS2,DX,DX2,AN,AN1
         INTEGER*2 N
         IF (X.GT.0.0) THEN
            GX=DLOG(X)
            N=N+1
```

```
      IF (N.EQ.1) THEN
         GS1=GX
         GS2=0.0
      ENDIF
      AN=FLOAT(N)
      AN1=FLOAT(N)-1.0
      DX=(GX-GS1)/AN
      DX2=DX*DX
      GS2=GS2+AN*AN1*DX2
      GS1=GS1+DX
   ENDIF
   RETURN
   END
```

```
      SUBROUTINE TRANSPOR
C
      INCLUDE 'INTERM.INC'
      INCLUDE 'MODEL.INC'
C
      DIMENSION XFE2(25),
     &DELGYP(25),DELGYA(25),NWW(25),
     &XFE3(25),XSO4(25),ALEQ(25),FE3EQ(25)
C
C
      IF(FLAG5 .EQ. 1. .AND. T .EQ. 1. .AND. I .EQ. 1. .AND.
     &IGUESS .EQ. 1)THEN
            OPEN(9,FILE="TRANSPOR.OUT")
            WRITE(9,10) 'T     ','I','CASE','PH      ','AFLUX   ','GYP     '
     &,'ALOH3  ','FEOH3  ','ALT     ','AL3     ','FE2T   ','FE3T   '
     &,'FE3     ','SO4     ','SO4T    ','CA      ','CACO3  ','POTAS  '
     &,'RPYR  ','PYR     ','ATOTAL ','AYEAR  '
10          FORMAT(' ',A10,2(A4,1X),19(A10,1X))
      ENDIF
C
C     INITIALIZING
C
C     NOTE THAT VRAIN IS IN L/MONTH
C
      IF ( T .EQ. 1) THEN
         ATOTAL(I,3) = 0.
         AYEAR(I,3) = 0.
         AFLUX(I,3) = 0.
         DELCAL(I) = 0.
         CASE(I) = '    '
      ENDIF
C
C     DISSOLUTION RATE ( MOLES/(M3 TAILINGS MONTH) )
C
      RPYR(I) = -RT(I,2)*ALPHAP(I,2)
C
      RSER(I) = 1.6E-3*(1.-0.11*PH(I,3))
      IF (RSER(I)  .LT. 0.) THEN
          RSER(I) = 0.
      ENDIF
C
      NWW(I) = NW(I)*1000.
C
      XFE2(I) = (0.46 - PO2(I,2)**(0.5))/0.48
      IF (XFE2(I) .LT. 0.) THEN
         XFE2(I) = 0.
      ENDIF
      XFE3(I) = (0.02 + PO2(I,2)**(0.5))/0.48
      XAL     =  1.0
      XSO4(I) = 2.0
C
C     CALCULATE THE RAIN EFFECTS
C     FOR THE "0" LAYER, IE. RAINWATER INPUT, THE ARRAY TERM ,I, WILL
C     BE SET EQUAL TO 25, A REFERENCE POINT TO AVOID ZERO ARRAY DIMENSIONS
C     FOR THE BOTTOM LAYER, DEEP SAT'D ZONE, THE INFLOWING WATER IS ONLY
```

```
C     10% OF THAT LEAVING THE MIXING ZONE AND HENCE I=24 IS USED.
C
      II = I-1
      IF ( II .EQ. 0) THEN
        II = 25.
      ENDIF
      IF (II .EQ. LAYSAT) THEN
        FRAC = 0.1
      ELSE
        FRAC = 1.0
      ENDIF
C
      POTAS(I,2) = VRAIN(II,M)*FRAC*POTAS(II,3)/VRAIN(I,M) +
     &             RSER(I)*VT(I)/VRAIN(I,M)
      FE2T(I,2)   = FE2T(II,3)*FRAC*VRAIN(II,M)/VRAIN(I,M) +
     &             XFE2(I)*RPYR(I)*VT(I)/VRAIN(I,M)
      CAT(I,2)    = CAT(II,3)*FRAC*VRAIN(II,M)/VRAIN(I,M)
      SO4T(I,2) =  SO4T(II,3)*FRAC*VRAIN(II,M)/VRAIN(I,M) +
     &            XSO4(I)*RPYR(I)*VT(I)/VRAIN(I,M)
C
      NO3T(I,2) = NO3T(II,3)*FRAC*VRAIN(II,M)/VRAIN(I,M)
C
C
C     CALCULATIONS FOR THE SATURATED ZONE
      IF ( I .GE. LC) THEN
         NO3T(I,2) = 0.
      ENDIF
C
C     CTT IS A MASS BALANCE ON TOTAL INORGANIC CARBON DUE TO
C     TRANSPORT.  THE ACTUAL EFFECT UPON CALCITE IS THEN TRACED BY
C     DOING A BALANCE BETWEEN CT AND CTT.
C
      XCT(I) = (DK1 + 2*10**(-PH(I,3)) )/(DK1 + 10**(-PH(I,3)) )
      IF ( CACO3(I,3) .GT. 0.) THEN
         CTT(I,2) = ( CTT(II,3)*FRAC*VRAIN(II,M) +
     &                XCT(I)*RPYR(I)*VT(I) )/VRAIN(I,M)
         DELCAL(I) = XCT(I)*RPYR(I)*DT
      ELSE
         CTT(I,2) = CTT(II,3)*FRAC*VRAIN(II,M)/VRAIN(I,M)
         DELCAL(I) = 0.
      END IF
C
C     MASS BALANCE FOR HE MIXING ZONE LAYER(i)=LAYSAT
      IF (I .GE. LC) THEN
C     UNITS OF REDFE3 ARE MOLES FET PER LITER PER MONTH
C
C
      IF ( FE3T(I,3) .LT. 1.E-25 ) THEN
         FE3T(I,3) = 1.E-25
      ENDIF
C
      REDFE3 = XKFE3*FE3T(I,3)*LIMO2/(LIMO2+PO2(I,2))*
     &        EXP(-CHEMEA/RG*(298.-TS(I,M))/(298.*TS(I,M)) )
C
        IF ( FEOH3(I,3) .GT. 0.) THEN
```

```
           YFEOH3  = REDFE3*NWW(I)*DT
           IF ( YFEOH3 .GT. FEOH3(I,3) ) THEN
              YYY = FEOH3(I,3)
              REDFE3 = REDFE3*YYY/YFEOH3
              YFEOH3 = YYY
           ENDIF
           FEOH3(I,3) = FEOH3(I,3) - YFEOH3
        ELSE
           XFEOH3 = REDFE3*DT
           IF (XFEOH3 .GT. FE3T(I,3)) THEN
              XXX = FE3T(I,3) - 1.E-18
              REDFE3 = XXX/XFEOH3
              XFEOH3 = XXX
           ENDIF
           FE3T(I,3) = FE3T(I,3) - XFEOH3
        ENDIF
        RPYR(I) = RPYR(I)- REDFE3/14.*NWW(I)*DT
        IF (RPYR(I) .LT. 0.) THEN
           RPYR(I) = 0.
        ENDIF
        FE2T(I,2) = FE2T(I,2) + REDFE3*DT*15./14.
        SO4T(I,2) = SO4T(I,2) + REDFE3*DT/7.
      ENDIF
C     THE END OF THE MIXING ZONE MASS BALANCE
C       GYPSUM PRECIPITATION/DISSOLUTION INITIAL CHECK
C
        SSFACT = 1.+CFESO4*F(3)*F(2)/F(1)*FE3(I,3)
     &            +CALSO4*F(3)*F(2)/F(1)*AL3(I,3)
     &            +10**(-PH(I,3))*F(2)/(CHSO4*F(1))
C
        A = SO4T(I,2) - CAT(I,2)
        B = KCASO4/F(2)**2*SSFACT
        CAEQU = (-A+(A**2+4*B)**(0.5))/2.
        SO4EQ = KCASO4/(F(2)**2*CAEQU)
        CA(I,2) = CAT(I,2)/(1.+CCASO4*F(2)**2*SO4(I,3) )
        IF (CAEQU .GT. CA(I,3)  .AND. GYP(I,3) .LE. 0.) THEN
           CAEQU = CA(I,2)
           SO4EQ = SO4T(I,2)/(SSFACT+CCASO4*F(2)**2*CA(I,3) )
        ENDIF
        SO4T(I,2) = SO4EQ*(SSFACT+CCASO4*F(2)**2*CAEQU)
        CATN = CAEQU*(1.+CCASO4*F(2)**2*SO4EQ)
        SO4(I,2) = SO4EQ
        CA(I,2) = CAEQU
        DELGYA(I) = CAT(I,2)- CATN
        CAT(I,2) = CATN
        CALIN = CAT(I,2)
C
C     CALCULATING CONCENTRATIONS AND PH AS A FUNCTION OF CASE
C
C     CASE 1.0  CALCITE PRESENT
      IF (CACO3(I,3) .GT. 0. ) THEN
C
C       CALCITE AND GYPSUM PRESENT
        IF ( GYP(I,3) .GT. 0.) THEN
C
```

```
          IF ( I .LT. LC) THEN
C           OPEN SYSTEM
            CASE(I) = 'C111'
          ELSE
C           CLOSED SYSTEM
            CASE(I) = 'C112'
          ENDIF
C
          CALL SPECIATION
C
        ELSE
C       CALCITE PRESENT,BUT GYPSUM ABSENT
          IF ( I .LT. LC) THEN
C           OPEN SYSTEM
            CASE(I) = 'C113'
          ELSE
C           CLOSED SYSTEM
            CASE(I) = 'C114'
C         MASS BALANCE FOR CT WHEN GYP NOT PRESENT
            IF (CACO3(I,3) .GT. 0.) THEN
              CT(I,2) = ( CT(II,3)*FRAC*VRAIN(II,M)+
     &                    XCT(I)*RPYR(I)*VT(I) )/VRAIN(I,M)
            ELSE
              CT(I,2) = CT(II,3)*FRAC*VRAIN(II,M)/VRAIN(I,M)
            END IF
          ENDIF
C
          CALL SPECIATION
C
          IF (I .LT. LC) THEN
              CA(I,2)=10**(-2*PH(I,2))*KCACO3/(DK1*DK2*
     &            KCO2*PCO2(I,2))
              CCAT = CA(I,2)*(1.+CCASO4*F(2)**2*SO4(I,2) )
              XCCA = (CCAT-CAT(I,2))*VRAIN(I,M)*DT/VT(I)
              IF (XCCA .GT. DELCAL(I)) THEN
                 DELCAL(I) = XCCA
              ENDIF
              CAT(I,2) = CCAT
              HCO3(I,2) = DK1*KCO2*PCO2(I,2)*10**(PH(I,2))/F(1)
              CT(I,2) = HCO3(I,2)*(10**(-PH(I,2)) + DK1)/DK1
          ELSE
              CA(I,2) = KCACO3*10**(-PH(I,2))*(10**(-PH(I,2))
     &                   +DK1)/( DK1*DK2*CT(I,2) )
              CAT(I,2) = CA(I,2)*(1.+CCASO4*F(2)*2*SO4(I,2) )
              HCO3(I,2) = DK1/(10**(-PH(I,2))+DK1)*CT(I,2)
          ENDIF
        ENDIF
C
C       PERFORMING IRON, ALUMINUM BALANCE
C
         FEFACT = (1.+CFEOH*F(3)/F(2)*10**PH(I,2) +
     &            CFEOH2*F(3)/F(1)*10**(2.*PH(I,2)) +
     &            CFEOH3*F(3)*10**(3.*PH(I,2))+
     &            CFESO4*F(3)*F(2)/F(1)*SO4(I,2))
         ALFACT = (1.+CALOH*F(3)/F(2)*10**PH(I,2)+
   &        CALOH2*F(3)/F(1)*10**(2.*PH(I,2))+
   &        CALOH3*F(3)*10**(3.*PH(I,2))+
   &        CALSO4*F(3)*F(2)/F(1)*SO4(I,2))
C
      IF (FEOH3(I,3) .GT. 0.) THEN
        FE3(I,2) = KFEOOH/F(3)*10**(-3.*PH(I,2))
        FE3T(I,2) = FE3(I,2)*FEFACT
        FEOH3(I,2) = FEOH3(I,3) +(FRAC*VRAIN(II,M)*FE3T(II,3)/VT(I)-
   &              VRAIN(I,M)*FE3T(I,2)/VT(I) +
   &              XFE3(I)*RPYR(I))*DT
      ELSE
        FE3T(I,2) = (FE3T(II,3)*FRAC*VRAIN(II,M) +
   &                XFE3(I)*RPYR(I)*VT(I))/VRAIN(I,M)
        FE3(I,2) = FE3T(I,2)/FEFACT
      ENDIF
C
      IF (ALOH3(I,3) .GT. 0.) THEN
        XZ = KBAS-10*PH(I,2)
        AL3(I,2) = (10**(XZ)/(F(2)*SO4(I,2))
   &                )**(0.25)/F(3)
        ALT(I,2) = AL3(I,2)*ALFACT
        ALOH3(I,2) = ALOH3(I,3) + (FRAC*VRAIN(II,M)*ALT(II,3)/VT(I)-
   &              VRAIN(I,M)*ALT(I,2)/VT(I)+XAL*RSER(I))*DT
      ELSE
        ALT(I,2) =  (ALT(II,3)*FRAC*VRAIN(II,M) +
   &             XAL*RSER(I)*VT(I))/VRAIN(I,M)
        AL3(I,2) = ALT(I,2)/ALFACT
     ENDIF
C
C    ******************************************************
C
C    CASES WHERE CALCITE IS ABSENT
C
C    SOLIDS BALANCE FOR BASALUMINITE AND FEOOH ARE DONE IN
C    THESE ROUTINES
C
C    CASE 2.0  BOTH FE(OH)3 AND AL(OH)3 ARE PRESENT
     ELSE IF (FEOH3(I,3) .GT. 0. .AND. ALOH3(I,3) .GT. 0.) THEN
C
     IF ( I .LT. LC) THEN
C      OPEN SYSTEM
       CASE(I) = 'C210'
     ELSE
C      CLOSED SYSTEM
       CASE(I) = 'C220'
     END IF
C
     CALL SPECIATION
C
      SFACT = ( 1.+(10**(-PH(I,2))*F(2))/(F(1)*CHSO4)+
   &         CALSO4*F(3)*F(2)/F(1)*AL3(I,2)+
   &         CFESO4*F(3)*F(2)/F(1)*FE3(I,2)+
   &         CCASO4*F(2)**2.*CA(I,2)      )
      SO4(I,2) = SO4T(I,2)/SFACT
C
```

```
         XZ = KBAS-10.*PH(I,2)
         AL3(I,2) =( 10**(XZ)/(SO4(I,2)*F(2))
     &              )**(0.25)/F(3)
C
         ALFACT = (1.+CALOH*F(3)/F(2)*10**PH(I,2)+
     &            CALOH2*F(3)/F(1)*10**(2.*PH(I,2))+
     &            CALOH3*F(3)*10**(3.*PH(I,2))+
     &            CALSO4*F(3)*F(2)/F(1)*SO4(I,2))
         ALT(I,2) = ALFACT*AL3(I,2)
C
         FE3SOL = KFEOOH/F(3)*10**(-3.*PH(I,2))
         FE3(I,2) = FE3SOL
C
         FEFACT = (1.+CFEOH*F(3)/F(2)*10**PH(I,2) +
     &            CFEOH2*F(3)/F(1)*10**(2.*PH(I,2)) +
     &            CFEOH3*F(3)*10**(3.*PH(I,2))+
     &            CFESO4*F(3)*F(2)/F(1)*SO4(I,2))
         FE3T(I,2) = FEFACT*FE3(I,2)
C
C
        FEOH3(I,2) = FEOH3(I,3) +(FRAC*VRAIN(II,M)*FE3T(II,3)/VT(I) -
     &               VRAIN(I,M)*FE3T(I,2)/VT(I) +
     &               XFE3(I)*RPYR(I))*DT
        ALOH3(I,2) = ALOH3(I,3) + (FRAC*VRAIN(II,M)*ALT(II,3)/VT(I)-
     &               VRAIN(I,M)*ALT(I,2)/VT(I)+XAL*RSER(I))*DT
C
C       IF ALOH3(I,2) IS ZERO THEN ALT MUST BE ALTERED TO REFLECT THIS.
C       THE FOLLOWING EQ. RECALCULATED ALT BASED ON C410 CONDITIONS.
C
        IF ( ALOH3(I,2) .LE. 0. ) THEN
           ALT(I,2) =  (ALT(II,3)*FRAC*VRAIN(II,M) +
     &              XAL*RSER(I)*VT(I))/VRAIN(I,M)
            AL3(I,2) = ALT(I,2)/ALFACT
        ENDIF
C
C     CASE 3  BOTH FE(OH)3 AND AL(OH)3 ARE ABSENT
      ELSE  IF (FEOH3(I,3) .LE. 0. .AND. ALOH3(I,3) .LE. 0.) THEN
C
        FE3T(I,2) = (FE3T(II,3)*FRAC*VRAIN(II,M) +
     &             XFE3(I)*RPYR(I)*VT(I))/VRAIN(I,M)
        ALT(I,2) =  (ALT(II,3)*FRAC*VRAIN(II,M) +
     &              XAL*RSER(I)*VT(I))/VRAIN(I,M)
C
        IF ( I .LT. LC) THEN
C         OPEN SYSTEM
          CASE(I) = 'C310'
        ELSE
C         CLOSED SYSTEM
          CASE(I) = 'C320'
        END IF
C
        CALL SPECIATION
C
        SFACT = ( 1.+(10**(-PH(I,2))*F(2))/(F(1)*CHSO4)+
     &        CALSO4*F(3)*F(2)/F(1)*AL3(I,2)+
     &       CFESO4*F(3)*F(2)/F(1)*FE3(I,2)+
     &       CCASO4*F(2)**2.*CA(I,2)      )
       SO4(I,2) = SO4T(I,2)/SFACT
C
C
C      CHECK ON SUPERSATURATION
C
       XZ = KBAS-10.*PH(I,2)
       ALEQ(I) = ( 10**(XZ)/(F(2)*SO4(I,2))
     &           )**0.25/F(3)*ALFACT
       IF (ALEQ(I) .LT. ALT(I,2)) THEN
          ALOH3(I,2) =  (ALT(I,2) - ALEQ(I))*NWW(I)
          ALT(I,2) = ALEQ(I)
       ELSE
          ALOH3(I,2) = 0.
       ENDIF
C
       FE3EQ(I) = KFEOOH/F(3)*10**(-3.*PH(I,2))*FEFACT
C
       IF (FE3EQ(I) .LT. FE3T(I,2)) THEN
         FEOH3(I,2) = (FE3T(I,2) - FE3EQ(I))*NWW(I)
         FE3T(I,2) = FE3EQ(I)
       ENDIF
C
C     CASE4  FE(OH)3 IS PRESENT BUT AL(OH)3 IS ABSENT
      ELSE IF (FEOH3(I,3) .GT. 0. .AND. ALOH3(I,3) .LE. 0.) THEN
C
       ALT(I,2) =  (ALT(II,3)*FRAC*VRAIN(II,M) +
     &             XAL*RSER(I)*VT(I))/VRAIN(I,M)
C
       IF ( I .LT. LC) THEN
C        OPEN SYSTEM
         CASE(I) = 'C410'
       ELSE
C        CLOSED SYSTEM
         CASE(I) = 'C420'
       END IF
C
       CALL SPECIATION
C
        SFACT = ( 1.+(10**(-PH(I,2))*F(2))/(F(1)*CHSO4)+
     &       CALSO4*F(3)*F(2)/F(1)*AL3(I,2)+
     &       CFESO4*F(3)*F(2)/F(1)*FE3(I,2)+
     &       CCASO4*F(2)**2.*CA(I,2)      )
        SO4(I,2) = SO4T(I,2)/SFACT
C
        FE3SOL = KFEOOH/F(3)*10**(-3.*PH(I,2))
        FE3(I,2) = FE3SOL
C
        FEFACT = (1.+CFEOH*F(3)/F(2)*10**PH(I,2) +
     &           CFEOH2*F(3)/F(1)*10**(2.*PH(I,2)) +
     &           CFEOH3*F(3)*10**(3.*PH(I,2))+
     &           CFESO4*F(3)*F(2)/F(1)*SO4(I,2))
        FE3T(I,2) = FEFACT*FE3(I,2)
C
```

```
        FEOH3(I,2) = FEOH3(I,3)+(FRAC*VRAIN(II,M)*FE3T(II,3)/VT(I)-
     &                VRAIN(I,M)*FE3T(I,2)/VT(I) +
     &               XFE3(I)*RPYR(I))*DT
C
C       CHECK ON SUPERSATURATION
C
        XZ = KBAS - 10.*PH(I,2)
        ALEQ(I) = (10**(XZ)/(F(2)*SO4(I,2))
     &            )**0.25/F(3)*ALFACT
        IF (ALEQ(I) .LT. ALT(I,2)) THEN
           ALOH3(I,2) = (ALT(I,2) - ALEQ(I))*NWW(I)
           ALT(I,2) = ALEQ(I)
        ENDIF
C
C
C     CASE 5  AL(OH)3 IS PRESENT BUT FE(OH)3 IS ABSENT
      ELSE
        FE3T(I,2) = (FRAC*VRAIN(II,M)*FE3T(II,3)+
     &             XFE3(I)*RPYR(I)*VT(I))/VRAIN(I,M)
C
        IF ( I .LT. LC) THEN
C         OPEN SYSTEM
          CASE(I) = 'C510'
        ELSE
C         CLOSED SYSTEM
          CASE(I) = 'C520'
        END IF
C
        CALL SPECIATION
C
         SFACT = ( 1.+(10**(-PH(I,2))*F(2))/(F(1)*CHSO4)+
     &         CALSO4*F(3)*F(2)/F(1)*AL3(I,2)+
     &         CFESO4*F(3)*F(2)/F(1)*FE3(I,2)+
     &         CCASO4*F(2)**2.*CA(I,2)       )
         SO4(I,2) = SO4T(I,2)/SFACT
C
         XZ = KBAS-10.*PH(I,2)
         AL3(I,2) =(10**(XZ)/(SO4(I,2)*F(2))
     &             )**(0.25)/F(3)
         ALFACT = (1.+CALOH*F(3)/F(2)*10**PH(I,2)+
     &            CALOH2*F(3)/F(1)*10**(2.*PH(I,2))+
     &            CALOH3*F(3)*10**(3.*PH(I,2))+
     &            CALSO4*F(3)*F(2)/F(1)*SO4(I,2))
         ALT(I,2) = ALFACT*AL3(I,2)
C
        ALOH3(I,2) = ALOH3(I,3) + (FRAC*VRAIN(II,M)*ALT(II,3)/VT(I)-
     &                VRAIN(I,M)*ALT(I,2)/VT(I)+XAL*RSER(I))*DT
C
C       CHECK ON SUPERSATURATION
C
        FE3EQ(I) = KFEOOH/F(3)*10**(-3.*PH(I,2))*( 1.
     &            +CFEOH*F(3)*10**(PH(I,2))/F(2) +
     &             CFEOH2*F(3)*10**(2.*PH(I,2))/F(1) +
     &             CFEOH3*F(3)*10**(3.*PH(I,2))+
     &             CFESO4*F(3)*F(2)*SO4(I,2)/F(1) )
```

```
          IF (FE3EQ(I) .LT. FE3T(I,2)) THEN
            FEOH3(I,2) = (FE3T(I,2) - FE3EQ(I))*NWW(I)
            FE3T(I,2) = FE3EQ(I)
            FE3(I,2) = FE3T(I,2)/FEFACT
          ENDIF
C
C
        END IF
C
C       RECALCULATIONS
C
C       THE FOLLOWING ALLOWS THE CALCULATED PH VALUE TO BE USED FOR
C       FINE TUNING
        IF (IGUESS .EQ. 1 .OR. IGUESS .EQ. 2) THEN
           PH(I,3) = PH(I,2)
           PO2(I,3) = PO2(I,2)
C          THE FOLLOWING IS USED TO AVOID BOUNDARY OSCILLATION
           IF (PO2(I,3) .EQ. 0.) THEN
              PO2(I,3) = 0.1
           ENDIF
          RETURN
        ENDIF
C       RECALCULATING THE CACO3 FOR BOTH THE SAT'DAND UNSAT'D ZONES
         IF (CACO3(I,3) .GT. 0. ) THEN
          IF ( I .GT. 1 ) THEN
           IF ( CACO3(II,3) .LE. 0.) THEN
             PART1 = FE3(II,3)*(  CFEOH*F(3)/F(2)*10**(PH(II,3)) +
     &               2.)*VRAIN(II,M)/VT(I)*DT
             PART2 = COEFAL*AL3(II,3)*(CALOH2*F(3)/F(1)*
     &               10**(2*PH(II,3)) + 2*CALOH*F(3)/F(2)*
     &               10**(PH(II,3)) + 3. )*VRAIN(II,M)/VT(I)*DT
             PART3   = XCT(I)*RPYR(I)*DT
             DELCAL(I) = 10**(-PH(I,2))*VRAIN(I,M)/VT(I)*DT + PART1 +
     &                   PART2 + PART3
             CAT(I,2) = CAT(II,3) + DELCAL(I)/NWW(I)
C           FOR THE SATURATED ZONE
             IF ( I .GE. LC ) THEN
                CT(I,2) = CT(II,3) + DELCAL(I)/NWW(I)
             ENDIF
C
          ENDIF
C        THE BOUNDRY LAYER CASE,LAYER(I) =1
         ELSE
           DELCAL(I) = XCT(I)*RPYR(I)*DT
         ENDIF
        ELSE
            DELCAL(I) = 0.0
        ENDIF
C
C       CACO3 FOR THE UNSATURATED ZONE
        CACO3(I,2) = CACO3(I,2) - DELCAL(I)
C
C       ALOH3 CALCULATIONS
C
C       THE 1.E-2 LIMIT ACCOUNTS FOR ANY SMALL PERTURBATION DUE TO FLOW
```

```
       IF (ALOH3(I,2) .LT. 1.E-2) THEN
          ALOH3(I,2) = 0.
       ENDIF
       IF (FEOH3(I,2) .LT. 1.E-2) THEN
          FEOH3(I,2) = 0.
       ENDIF
C
C     GYPSUM PRECIPITATION/DISSOLUTION
C
        IF (FEOH3(I,2) .LT. 1.E-2) THEN
          FEOH3(I,2) = 0.
       ENDIF
C
C     GYPSUM PRECIPITATION/DISSOLUTION
C
        SSFACT = 1.+CFESO4*F(3)*F(2)/F(1)*FE3(I,2)
     &             +CALSO4*F(3)*F(2)/F(1)*AL3(I,2)
     &             +10**(-PH(I,2))*F(2)/(CHSO4*F(1))
        A = SO4T(I,2) - CAT(I,2)
        B = KCASO4/F(2)**2*SSFACT
        CAEQU = (-A+(A**2+4*B)**(0.5))/2.
        SO4EQ = KCASO4/(F(2)**2*CAEQU)
        CA(I,2) = CAT(I,2)/(1.+CCASO4*F(2)**2*SO4(I,2) )
        IF (CAEQU .GT. CA(I,2)  .AND. GYP(I,3) .LE. 0.) THEN
           CAEQU = CA(I,2)
           SO4EQ = SO4T(I,2)/(SSFACT+CCASO4*F(2)**2*CA(I,2) )
        ENDIF
        SO4T(I,2) = SO4EQ*(SSFACT+CCASO4*F(2)**2*CAEQU)
        CATN = CAEQU*(1.+CCASO4*F(2)**2*SO4EQ)
        SO4(I,2) = SO4EQ
        CA(I,2) = CAEQU
        DELGYP(I) = CALIN - CATN
        CAT(I,2) = CATN
C
C     CHECKING FOR NEGATIVE PH
      IF (PH(I,2) .LT. 0.) THEN
         CALL ERROR (52,0)
      ENDIF
C
C     SOLIDS INVENTORY   (MOL/M3 TAILINGS)
      SER(I,2) = SER(I,3) -RSER(I)*DT
      GYP(I,2)= GYP(I,3) + (DELGYP(I) + DGYP(I,2)+
     &          DELGYA(I))*VRAIN(I,M)*DT/VT(I)
C
C     ACID FLUX
C
C     MONTHLY
C     ( CONC. IN MOL/L  ; AFLUX IN MOL/(M2 MTH) ; INFILT IN M/MTH )
       AFLUX(I,2) = (2*SO4T(I,2)+HCO3(I,2)-2*CAT(I,2)-POTAS(I,2)
     &        )*1000.*INFILT(I,M)
C
C     YEARLY ( MOL/M2 YEAR )
      IF ( M .EQ. 1) THEN
        AYEAR(I,2) = AFLUX(I,2)
      ELSE
```

```
        AYEAR(I,2) = AFLUX(I,2) + AYEAR(I,3)
      ENDIF
C
C     TOTAL OF ACID FLUX (MOL/M2 MTH)
       ATOTAL(I,2) = ATOTAL(I,3) + AFLUX(I,2)
C
       IF (GYP(I,2) .LT. 0.) THEN
          GYP(I,2) = 0.
       ENDIF
       IF (CACO3(I,2) .LT. 0.) THEN
          CACO3(I,2) = 0.
       ENDIF
       IF (SER(I,2) .LT. 0.) THEN
           SER(I,2) = 0.
       ENDIF
       IF (AFLUX(I,2) .LT. 0.) THEN
           AFLUX(I,2) = 0.
       ENDIF

C       THE FOLLOWING IS THE RENAMING OF VARIABLE FROM PRESENT TO PAST
C       AND ESTIMATING THE NEXT PH
        IF (I .EQ. LAYER ) THEN
C
         IF ( T .NE. NYEARS) THEN
           DO 900  IJ = 1,LAYER
C
C     SETING UP FOR THE NEXT MONTHLY TIME STEP
C     ADJUSTING THE INITIAL GUESS IF A "CASE" CHANGE OCCURS
C
       IF ( M .EQ. MONTH .AND. FLAG5 .EQ. 1. .AND.
     &IGUESS .EQ. 3) THEN
             WRITE(9,975) T,IJ,CASE(IJ),PH(IJ,2),AFLUX(IJ,2),GYP(IJ,2),
     &       ALOH3(IJ,2),FEOH3(IJ,2),ALT(IJ,2),AL3(IJ,2),FE2T(IJ,2),
     &    FE3T(IJ,2),FE3(IJ,2),SO4(IJ,2),SO4T(IJ,2),CA(IJ,2),CACO3(IJ,2)
     &      ,POTAS(IJ,2),RPYR(IJ),PYR(IJ,2),ATOTAL(IJ,2),AYEAR(IJ,2)
975         FORMAT(' ',E10.4,1X,I3,1X,A4,1X,19(E10.4,1X))
        ENDIF
C
           MMM = M+1
           IF (MMM .EQ. 13) THEN
              MMM = 1
           ENDIF
C
C         CALCITE PRESENT CASES
C         CASES 1.11,1.12,1.13, AND 1.14
          IF (CACO3(IJ,2) .GT. 0.) THEN
            PH(IJ,3) = 6.5
C
C         CALCITE ABSENT CASES
C         CASES 2.1,2.2,3.1,AND 3.2
          ELSE   IF (ALOH3(IJ,2) .GT. 0.) THEN
C
              IF (MMM .EQ. 1 .OR. MMM .EQ. 2 .OR. MMM .EQ. 3 .OR. MMM
     &            .EQ. 12) THEN
                  PH(IJ,3) = 4.0
            ELSE
                PH(IJ,3) = 3.5
            ENDIF
C
C       CASE 410 OR 510
        ELSE
            IF (MMM .EQ. 1 .OR. MMM .EQ. 2 .OR. MMM .EQ. 3 .OR. MMM
     &          .EQ. 12) THEN
                PH(IJ,3) = 2.0
            ELSE
                PH(IJ,3) = 2.5
            ENDIF
        ENDIF
C
C       IF THE PYRITE HAS BEEN DEPLETED THEN
          IF ( PYR(I,2) .LE. 0.) THEN
               PYR(I,2) = 0.
               PH(IJ,3) = 6.
          ENDIF
C
C       SETTING  INITIAL OXYGEN GUESS
           PO2(IJ,3) = 1.0
C
C       WHEN CACO3 IS PRESENT THE CO2 LEVEL RISES
          PCO2(IJ,3) = PCO2(IJ,2)
          IF (CACO3(IJ,2) .GT. 0.) THEN
            PCO2(IJ,2) = 3.2E-4*100.
          ELSE
            PCO2(IJ,2) = 3.2E-4
          ENDIF
          PCO2(IJ,3) = PCO2(IJ,2)
C
                     AFLUX(IJ,3) = AFLUX(IJ,2)
                     P(IJ,3) = P(IJ,2)
                     KC(IJ,3) = KC(IJ,2)
                     R1(IJ,3) = R1(IJ,2)
                     R2(IJ,3) = R2(IJ,2)
                     RO2(IJ,3) = RO2(IJ,2)
                     AS(IJ,3) = AS(IJ,2)
                     PYR(IJ,3) = PYR(IJ,2)
                     SA(IJ,3) = SA(IJ,2)
                     ALPHAP(IJ,3) = ALPHAP(IJ,2)
                     RAD(IJ,3) = RAD(IJ,2)
                     R1B(IJ,3) = R1B(IJ,2)
                     NP(IJ,3) = NP(IJ,2)
                     COX(IJ,3) = COX(IJ,2)
                     HCO3(IJ,3) = HCO3(IJ,2)
                     CA(IJ,3) = CA(IJ,2)
                     CT(IJ,3) = CT(IJ,2)
                     FE2(IJ,3) = FE2(IJ,2)
                     CAT(IJ,3) = CAT(IJ,2)
                     SO4(IJ,3) = SO4(IJ,2)
                     FE2T(IJ,3) = FE2T(IJ,2)
                     SO4T(IJ,3) = SO4T(IJ,2)
                     SULF(IJ,3) = SULF(IJ,2)
                     FE3T(IJ,3) = FE3T(IJ,2)
                     ALUM(IJ,3) = ALUM(IJ,2)
                     IRON(IJ,3) = IRON(IJ,2)
                     POTAS(IJ,3) = POTAS(IJ,2)
                     CACO3(IJ,3) = CACO3(IJ,2)
                     CTT(IJ,3) = CTT(IJ,2)
                     NO3T(IJ,3) = NO3T(IJ,2)
                     ALOH3(IJ,3) = ALOH3(IJ,2)
                     SER(IJ,3) = SER(IJ,2)
                     FEOH3(IJ,3) = FEOH3(IJ,2)
                     GYP(IJ,3) = GYP(IJ,2)
                     AL3(IJ,3) = AL3(IJ,2)
                     FE3(IJ,3) = FE3(IJ,2)
                     ALT(IJ,3) = ALT(IJ,2)
                   ATOTAL(IJ,3) = ATOTAL(IJ,2)
                    AYEAR(IJ,3) = AYEAR(IJ,2)
900                CONTINUE
              ENDIF
         ENDIF
C
      RETURN
      END
```

APPENDIX C

SAMPLE INPUT FILES

APPENDIX C SAMPLE INPUT FILES

C.1 INPUTP.DAT

The probabilistic input file, INPUTP.DAT, shown in Table C.1 employs 50 trials to simulate the upper and lower limits of acid generation. Each trial is for a 186 month period and employs 12 soil layers with a water table located at a depth of 4.0 metres. The duration of this probabilistic run is approximately 15 hours (20 minutes per trial).

C.2 INPUTD.DAT

The deterministic input.file, INPUTD.DAT, is shown Table C.2. In the deterministic simulation, acid generation is predicted for a period of 246 months. The tailings is divided into 22 layers with the water table located at 4.0 m. The duration of the deterministic run is approximately 60 minutes when no detailed results files are required.

Table C.1 Probabilistic Data File (INPUTP.DAT)

```
PROBABILISTIC ANALYSIS: INPUTP.DAT
N Y
RES.PRB
KEY.PRB
184 0   0
0913566091  50
186.
FLAG1  N 1  N     0.
FLAG2  N 1  N     0.
FLAG3  N 1  N     0.
FLAG4  N 1  N     0.
FLAG5  N 1  N     0.
FLAG6  N 1  N     0.
MONTH  N 1  N     6.
BIOEA  N 6  N  10000.    11700.    16300.
CHEMEA N 1  N  13300.
BIOMAX N 4  N  11.5      14.5
LIMP   N 1  N  1.29E-3
BIOXP  N 3  N  1.6E-3    1.7       3.2E-4     7.8E-3
BIOYXS N 6  N  2.5       3.2       4.2
LIMO2  N 1  N  0.01
XKFE3  N 6  N  0.005     0.01      0.05
XPYR   N 4  N  0.048     0.072
XGYP   N 4  N  0.04      0.06
XFEOH3 N 4  N  0.0025    0.0057
XALOH3 N 4  N  0.0014    0.0032
XSER   N 4  N  0.11      0.16
XCACO3 N 4  N  0.0       0.001
SATCT  N 4  N  1.E-3     1.E-2
BULKD  N 1  N    1.3E+6
ATAIL  N 1  N    3.E+7
MOLARD N 1  N    41670.
ALPHA  N 1  N    0.9
BETA   N 1  N    1.8
COEFX  N 1  N    2.0
COEFY  N 1  N    -1.0
RADMAX N 1  N   1.25E-4
CHEMKC N 6  N  1.18E+5   2.36E+6   4.72E+7
COEFAL N 6  N  0.01      0.075     0.6
LAYER  N 1  N     12.
COVER  N 1  N     0.
LAYSAT N 1  N     11.
HENRY  N 1  N     23.6
KCO2   N 1  N     0.053
COEFAO N 1  N     20.
AVGTEM N 1  N     283.
COEFPS N 1  N     0.1
COEFDD N 1  N     2.0
WATTAB N 1  N     4.0
VRFRAC N 1  N     0.2
LA(1)  N 4  N     0.68   0.78
LA(2)  N 4  N     0.68   0.78
```

Table C.1 continued

LA(3)	N	4	N	0.68	0.78		
LA(4)	N	4	N	0.68	0.78		
LA(5)	N	4	N	0.68	0.78		
LA(6)	N	4	N	0.68	0.78		
LA(7)	N	4	N	0.68	0.78		
LA(8)	N	4	N	0.68	0.78		
LA(9)	N	4	N	0.68	0.78		
LA(10)	N	4	N	0.68	0.78		
LA(11)	N	4	N	0.68	0.78		
LA(12)	N	4	N	0.68	0.78		
LA(13)	N	1	N	0.			
LA(14)	N	1	N	0.			
LA(15)	N	1	N	0.			
LA(16)	N	1	N	0.			
LA(17)	N	1	N	0.			
LA(18)	N	1	N	0.			
LA(19)	N	1	N	0.			
LA(20)	N	1	N	0.			
LA(21)	N	1	N	0.			
LA(22)	N	1	N	0.			
NT(1)	N	6	N	0.45	0.50	0.55	
NT(2)	N	6	N	0.45	0.50	0.55	
NT(3)	N	6	N	0.45	0.50	0.55	
NT(4)	N	6	N	0.45	0.50	0.55	
NT(5)	N	6	N	0.45	0.50	0.55	
NT(6)	N	6	N	0.45	0.50	0.55	
NT(7)	N	6	N	0.45	0.50	0.55	
NT(8)	N	6	N	0.45	0.50	0.55	
NT(9)	N	6	N	0.45	0.50	0.55	
NT(10)	N	6	N	0.45	0.50	0.55	
NT(11)	N	6	N	0.45	0.50	0.55	
NT(12)	N	6	N	0.45	0.50	0.55	
NT(13)	N	1	N	0.			
NT(14)	N	1	N	0.			
NT(15)	N	1	N	0.			
NT(16)	N	1	N	0.			
NT(17)	N	1	N	0.			
NT(18)	N	1	N	0.			
NT(19)	N	1	N	0.			
NT(20)	N	1	N	0.			
NT(21)	N	1	N	0.			
NT(22)	N	1	N	0.			
NR(1)	N	2	N	0.08	0.01	0.05	0.11
NR(2)	N	2	N	0.08	0.01	0.05	0.11
NR(3)	N	2	N	0.08	0.01	0.05	0.11
NR(4)	N	2	N	0.08	0.01	0.05	0.11
NR(5)	N	2	N	0.08	0.01	0.05	0.11
NR(6)	N	2	N	0.08	0.01	0.05	0.11
NR(7)	N	2	N	0.08	0.01	0.05	0.11
NR(8)	N	2	N	0.08	0.01	0.05	0.11
NR(9)	N	2	N	0.08	0.01	0.05	0.11
NR(10)	N	2	N	0.08	0.01	0.05	0.11
NR(11)	N	2	N	0.08	0.01	0.05	0.11

Table C.1 continued

NR(12)	N	2	N	0.08	0.01	0.05	0.11
NR(13)	N	1	N	0.			
NR(14)	N	1	N	0.			
NR(15)	N	1	N	0.			
NR(16)	N	1	N	0.			
NR(17)	N	1	N	0.			
NR(18)	N	1	N	0.			
NR(19)	N	1	N	0.			
NR(20)	N	1	N	0.			
NR(21)	N	1	N	0.			
NR(22)	N	1	N	0.			
HE(1)	N	6	N	-1.5	-0.5	-0.05	
HE(2)	N	6	N	-1.5	-0.5	-0.05	
HE(3)	N	6	N	-1.5	-0.5	-0.05	
HE(4)	N	6	N	-1.5	-0.5	-0.05	
HE(5)	N	6	N	-1.5	-0.5	-0.05	
HE(6)	N	6	N	-1.5	-0.5	-0.05	
HE(7)	N	6	N	-1.5	-0.5	-0.05	
HE(8)	N	6	N	-1.5	-0.5	-0.05	
HE(9)	N	6	N	-1.5	-0.5	-0.05	
HE(10)	N	6	N	-1.5	-0.5	-0.05	
HE(11)	N	6	N	-1.5	-0.5	-0.05	
HE(12)	N	6	N	-1.5	-0.5	-0.05	
HE(13)	N	1	N	0.			
HE(14)	N	1	N	0.			
HE(15)	N	1	N	0.			
HE(16)	N	1	N	0.			
HE(17)	N	1	N	0.			
HE(18)	N	1	N	0.			
HE(19)	N	1	N	0.			
HE(20)	N	1	N	0.			
HE(21)	N	1	N	0.			
HE(22)	N	1	N	0.			
DX(1)	N	1	N	0.4			
DX(2)	N	1	N	0.4			
DX(3)	N	1	N	0.4			
DX(4)	N	1	N	0.4			
DX(5)	N	1	N	0.4			
DX(6)	N	1	N	0.4			
DX(7)	N	1	N	0.4			
DX(8)	N	1	N	0.4			
DX(9)	N	1	N	0.4			
DX(10)	N	1	N	0.4			
DX(11)	N	1	N	0.4			
DX(12)	N	1	N	0.4			
DX(13)	N	1	N	0.			
DX(14)	N	1	N	0.			
DX(15)	N	1	N	0.			
DX(16)	N	1	N	0.			
DX(17)	N	1	N	0.			
DX(18)	N	1	N	0.			
DX(19)	N	1	N	0.			
DX(20)	N	1	N	0.			

Table C.1 continued

DX(21)	N	1	N	0.		
DX(22)	N	1	N	0.		
VR(1)	N	6	N	0.001	0.005	0.01	
VR(2)	N	6	N	0.001	0.005	0.01	
VR(3)	N	6	N	0.001	0.005	0.01	
VR(4)	N	6	N	0.018	0.09	0.18	
VR(5)	N	6	N	0.014	0.07	0.14	
VR(6)	N	6	N	0.006	0.03	0.06	
VR(7)	N	6	N	0.004	0.02	0.04	
VR(8)	N	6	N	0.006	0.03	0.06	
VR(9)	N	6	N	0.01	0.05	0.1	
VR(10)	N	6	N	0.01	0.05	0.1	
VR(11)	N	6	N	0.008	0.04	0.08	
VR(12)	N	6	N	0.001	0.005	0.01	
CHSO4	N	1	N	1.26E-2			
CCASO4	N	1	N	316.23			
CALSO4	N	1	N	1047.13			
CFEOH	N	1	N	6.46E-3			
CFEOH2	N	1	N	2.14E-6			
CFESO4	N	1	N	8317.64			
CFEOH3	N	1	N	1.E-12			
CALOH3	N	1	N	1.E-15			
F(1)	N	6	N	0.67	0.84	1.01	
F(2)	N	6	N	0.399	0.499	0.599	
F(3)	N	6	N	0.181	0.201	0.221	
KCASO4	N	3	N	2.45E-5	1.05	2.14E-5	2.75E-5
DK1	N	1	N	5.012E-7			
DK2	N	1	N	5.012E-11			
KCACO3	N	3	N	4.48E-9	1.05	3.89E-9	5.13E-9
KFEOOH	N	3	N	39.81	3.16	1.27	1.27E+3
CALOH2	N	1	N	5.0E-10			
CALOH	N	1	N	1.07E-5			
KBAS	N	3	N	22.7	1.02	21.7	23.7

TABLE C.2 Deterministic Data File (INPUTD.DAT)

```
DETERMINISTIC ANALYSIS: INPUTD.DAT
N N
RES.NOM
KEY.NOM
184      0   0
0913566091   1
246.
FLAG1   N 1  N      1.
FLAG2   N 1  N      1.
FLAG3   N 1  N      1.
FLAG4   N 1  N      1.
FLAG5   N 1  N      1.
FLAG6   N 1  N      1.
MONTH   N 1  N      6.
BIOEA   N 1  N      11700.
CHEMEA  N 1  N      13300.
BIOMAX  N 1  N      13.0
LIMP    N 1  N     1.29E-3
BIOXP   N 1  N     1.6E-3
BIOYXS  N 1  N      3.2
LIMO2   N 1  N      0.01
XKFE3   N 1  N     0.01
XPYR    N 1  N     0.06
XGYP    N 1  N     0.05
XFEOH3  N 1  N     0.0041
XALOH3  N 1  N     0.0023
XSER    N 1  N     0.136
XCACO3  N 1  N     0.0005
SATCT   N 1  N     .0055
BULKD   N 1  N     1.3E+6
ATAIL   N 1  N      3.E+7
MOLARD  N 1  N      41670.
ALPHA   N 1  N      0.9
BETA    N 1  N      1.8
COEFX   N 1  N      2.0
COEFY   N 1  N      -1.0
RADMAX  N 1  N     1.25E-4
CHEMKC  N 1  N      2.3E6
COEFAL  N 1  N      0.075
LAYER   N 1  N      22.
COVER   N 1  N      0.
LAYSAT  N 1  N      21.
HENRY   N 1  N      23.6
KCO2    N 1  N      0.053
COEFAO  N 1  N      20.
AVGTEM  N 1  N      283.
COEFPS  N 1  N      0.1
COEFDD  N 1  N      2.0
WATTAB  N 1  N      4.0
VRFRAC  N 1  N      0.2
LA(1)   N 1  N      0.73
LA(2)   N 1  N      0.73
LA(3)   N 1  N      0.73
LA(4)   N 1  N      0.73
LA(5)   N 1  N      0.73
```

Table C.2 continued

LA(3)	N 1	N	0.73
LA(4)	N 1	N	0.73
LA(5)	N 1	N	0.73
LA(6)	N 1	N	0.73
LA(7)	N 1	N	0.73
LA(8)	N 1	N	0.73
LA(9)	N 1	N	0.73
LA(10)	N 1	N	0.73
LA(11)	N 1	N	0.73
LA(12)	N 1	N	0.73
LA(13)	N 1	N	0.73
LA(14)	N 1	N	0.73
LA(15)	N 1	N	0.73
LA(16)	N 1	N	0.73
LA(17)	N 1	N	0.73
LA(18)	N 1	N	0.73
LA(19)	N 1	N	0.73
LA(20)	N 1	N	0.73
LA(21)	N 1	N	0.73
LA(22)	N 1	N	0.73
NT(1)	N 1	N	0.5
NT(2)	N 1	N	0.5
NT(3)	N 1	N	0.5
NT(4)	N 1	N	0.5
NT(5)	N 1	N	0.5
NT(6)	N 1	N	0.5
NT(7)	N 1	N	0.5
NT(8)	N 1	N	0.5
NT(9)	N 1	N	0.5
NT(10)	N 1	N	0.5
NT(11)	N 1	N	0.5
NT(12)	N 1	N	0.5
NT(13)	N 1	N	0.5
NT(14)	N 1	N	0.5
NT(15)	N 1	N	0.5
NT(16)	N 1	N	0.5
NT(17)	N 1	N	0.5
NT(18)	N 1	N	0.5
NT(19)	N 1	N	0.5
NT(20)	N 1	N	0.5
NT(21)	N 1	N	0.5
NT(22)	N 1	N	0.5
NR(1)	N 1	N	0.08
NR(2)	N 1	N	0.08
NR(3)	N 1	N	0.08
NR(4)	N 1	N	0.08
NR(5)	N 1	N	0.08
NR(6)	N 1	N	0.08
NR(7)	N 1	N	0.08
NR(8)	N 1	N	0.08
NR(9)	N 1	N	0.08
NR(10)	N 1	N	0.08
NR(11)	N 1	N	0.08

Table C.2 continued

NR(12)	N	1	N	0.08
NR(13)	N	1	N	0.08
NR(14)	N	1	N	0.08
NR(15)	N	1	N	0.08
NR(16)	N	1	N	0.08
NR(17)	N	1	N	0.08
NR(18)	N	1	N	0.08
NR(19)	N	1	N	0.08
NR(20)	N	1	N	0.08
NR(21)	N	1	N	0.08
NR(22)	N	1	N	0.08
HE(1)	N	1	N	-0.5
HE(2)	N	1	N	-0.5
HE(3)	N	1	N	-0.5
HE(4)	N	1	N	-0.5
HE(5)	N	1	N	-0.5
HE(6)	N	1	N	-0.5
HE(7)	N	1	N	-0.5
HE(8)	N	1	N	-0.5
HE(9)	N	1	N	-0.5
HE(10)	N	1	N	-0.5
HE(11)	N	1	N	-0.5
HE(12)	N	1	N	-0.5
HE(13)	N	1	N	-0.5
HE(14)	N	1	N	-0.5
HE(15)	N	1	N	-0.5
HE(16)	N	1	N	-0.5
HE(17)	N	1	N	-0.5
HE(18)	N	1	N	-0.5
HE(19)	N	1	N	-0.05
HE(20)	N	1	N	-0.05
HE(21)	N	1	N	-0.05
HE(22)	N	1	N	-0.05
DX(1)	N	1	N	0.2
DX(2)	N	1	N	0.2
DX(3)	N	1	N	0.2
DX(4)	N	1	N	0.2
DX(5)	N	1	N	0.2
DX(6)	N	1	N	0.2
DX(7)	N	1	N	0.2
DX(8)	N	1	N	0.2
DX(9)	N	1	N	0.2
DX(10)	N	1	N	0.2
DX(11)	N	1	N	0.2
DX(12)	N	1	N	0.2
DX(13)	N	1	N	0.2
DX(14)	N	1	N	0.2
DX(15)	N	1	N	0.2
DX(16)	N	1	N	0.2
DX(17)	N	1	N	0.2
DX(18)	N	1	N	0.2
DX(19)	N	1	N	0.2
DX(20)	N	1	N	0.2

Table C.2 continued

DX(21)	N	1	N	0.2
DX(22)	N	1	N	0.2
VR(1)	N	1	N	0.005
VR(2)	N	1	N	0.005
VR(3)	N	1	N	0.005
VR(4)	N	1	N	0.09
VR(5)	N	1	N	0.07
VR(6)	N	1	N	0.03
VR(7)	N	1	N	0.02
VR(8)	N	1	N	0.03
VR(9)	N	1	N	0.05
VR(10)	N	1	N	0.05
VR(11)	N	1	N	0.04
VR(12)	N	1	N	0.005
CHSO4	N	1	N	1.26E-2
CCASO4	N	1	N	316.23
CALSO4	N	1	N	1047.13
CFEOH	N	1	N	6.46E-3
CFEOH2	N	1	N	2.14E-6
CFESO4	N	1	N	8317.64
CFEOH3	N	1	N	1.E-12
CALOH3	N	1	N	1.E-15
F(1)	N	1	N	0.840
F(2)	N	1	N	0.499
F(3)	N	1	N	0.201
KCASO4	N	1	N	2.45E-5
DK1	N	1	N	5.012E-7
DK2	N	1	N	5.012E-11
KCACO3	N	1	N	4.48E-9
KFEOOH	N	1	N	39.81
CALOH2	N	1	N	5.0E-10
CALOH	N	1	N	1.07E-5
KBAS	N	1	N	22.7

APPENDIX D

SAMPLE OUTPUT FILES

APPENDIX D SAMPLE OF OUTPUT FILES

Table D.1 to D.8 contain sample output files. The summary statistic files for the probalistic (KEY.PRB) and deterministic (KEY.NOM) simulations are presented in tables D.1 and D.2, respectively. Tables D.3 to D.8 present the detailed outputs for the individual modules: initial.out, kinetic.out, oxygen.out, pyrite.out, transpor.out, speciati.out.

Table D.1 KEY.PRB

```
FILE CREATED 03/20/87 AT 08:24:41
 PROBABILISTIC ANALYSIS: INPUTP.DAT
 NUMBER OF TRIALS:     50
     PARAMETER          LOCATION  YEAR MONTH    MEAN      STD DEV   GEOM MEAN   GEOM SD    MINIMUM    MAXIMUM   SKEWNESS   KURTOSIS
  1     PH                  1       1    6   0.624E+01  0.144E+01  0.603E+01  0.133E+01  0.350E+01  0.722E+01  -.133E+01  0.281E+01
  2     PH                  1       2    6   0.416E+01  0.126E+01  0.401E+01  0.129E+01  0.350E+01  0.691E+01  0.166E+01  0.378E+01
  3     PH                  1       3    6   0.360E+01  0.111E+01  0.344E+01  0.135E+01  0.157E+01  0.684E+01  0.144E+01  0.637E+01
  4     PH                  1       4    6   0.303E+01  0.931E+00  0.289E+01  0.136E+01  0.157E+01  0.671E+01  0.662E+00  0.587E+01
  5     PH                  1       5    6   0.253E+01  0.926E+00  0.240E+01  0.136E+01  0.155E+01  0.671E+01  0.210E+01  0.930E+01
  6     PH                  1       6    6   0.224E+01  0.590E+00  0.218E+01  0.127E+01  0.140E+01  0.373E+01  0.142E+01  0.449E+01
  7     PH                  1       7    6   0.219E+01  0.566E+00  0.213E+01  0.126E+01  0.140E+01  0.374E+01  0.161E+01  0.527E+01
  8     PH                  1       8    6   0.210E+01  0.472E+00  0.206E+01  0.122E+01  0.145E+01  0.369E+01  0.201E+01  0.781E+01
  9     PH                  1       9    6   0.215E+01  0.680E+00  0.208E+01  0.126E+01  0.145E+01  0.590E+01  0.382E+01  0.204E+02
 10     PH                  1      10    6   0.211E+01  0.646E+00  0.205E+01  0.124E+01  0.145E+01  0.590E+01  0.439E+01  0.255E+02
 11     PH                  1      11    6   0.211E+01  0.641E+00  0.205E+01  0.124E+01  0.145E+01  0.590E+01  0.447E+01  0.262E+02
 12     PH                  1      12    6   0.223E+01  0.909E+00  0.212E+01  0.133E+01  0.146E+01  0.590E+01  0.316E+01  0.124E+02
 13     PH                  1      13    6   0.240E+01  0.115E+01  0.223E+01  0.142E+01  0.146E+01  0.591E+01  0.218E+01  0.641E+01
 14     PH                  1      14    6   0.262E+01  0.138E+01  0.238E+01  0.151E+01  0.146E+01  0.617E+01  0.162E+01  0.402E+01
 15     PH                  1      15    6   0.305E+01  0.163E+01  0.269E+01  0.162E+01  0.161E+01  0.617E+01  0.880E+00  0.200E+01
 16     PH                  1      16    6   0.331E+01  0.172E+01  0.291E+01  0.166E+01  0.161E+01  0.617E+01  0.534E+00  0.149E+01
 17     PH                  5       1    6   0.667E+01  0.775E+00  0.661E+01  0.116E+01  0.358E+01  0.697E+01  -.368E+01  0.146E+02
 18     PH                  5       2    6   0.597E+01  0.147E+01  0.575E+01  0.133E+01  0.358E+01  0.719E+01  -.971E+00  0.196E+01
 19     PH                  5       3    6   0.495E+01  0.161E+01  0.470E+01  0.137E+01  0.355E+01  0.715E+01  0.413E+00  0.118E+01
 20     PH                  5       4    6   0.426E+01  0.134E+01  0.409E+01  0.132E+01  0.209E+01  0.711E+01  0.137E+01  0.323E+01
 21     PH                  5       5    6   0.380E+01  0.100E+01  0.369E+01  0.126E+01  0.207E+01  0.701E+01  0.205E+01  0.802E+01
 22     PH                  5       6    6   0.341E+01  0.789E+00  0.332E+01  0.128E+01  0.167E+01  0.671E+01  0.565E+00  0.809E+01
 23     PH                  5       7    6   0.317E+01  0.732E+00  0.308E+01  0.130E+01  0.167E+01  0.381E+01  -.824E+00  0.179E+01
 24     PH                  5       8    6   0.286E+01  0.824E+00  0.274E+01  0.135E+01  0.165E+01  0.381E+01  -.726E-01  0.112E+01
 25     PH                  5       9    6   0.269E+01  0.819E+00  0.257E+01  0.135E+01  0.165E+01  0.375E+01  0.321E+00  0.122E+01
 26     PH                  5      10    6   0.246E+01  0.748E+00  0.236E+01  0.132E+01  0.163E+01  0.374E+01  0.923E+00  0.210E+01
 27     PH                  5      11    6   0.235E+01  0.687E+00  0.227E+01  0.129E+01  0.164E+01  0.374E+01  0.129E+01  0.299E+01
 28     PH                  5      12    6   0.217E+01  0.550E+00  0.212E+01  0.124E+01  0.146E+01  0.375E+01  0.204E+01  0.633E+01
 29     PH                  5      13    6   0.213E+01  0.510E+00  0.209E+01  0.122E+01  0.146E+01  0.376E+01  0.230E+01  0.785E+01
 30     PH                  5      14    6   0.201E+01  0.327E+00  0.199E+01  0.115E+01  0.147E+01  0.377E+01  0.309E+01  0.180E+02
 31     PH                  5      15    6   0.200E+01  0.327E+00  0.198E+01  0.115E+01  0.147E+01  0.378E+01  0.325E+01  0.189E+02
 32     PH                  5      16    6   0.200E+01  0.322E+00  0.198E+01  0.115E+01  0.146E+01  0.379E+01  0.340E+01  0.201E+02
 33     PH                 11       1    6   0.685E+01  0.229E+00  0.684E+01  0.103E+01  0.650E+01  0.736E+01  0.729E+00  0.254E+01
 34     PH                 11       2    6   0.716E+01  0.634E+00  0.712E+01  0.112E+01  0.351E+01  0.822E+01  -.372E+01  0.232E+02
 35     PH                 11       3    6   0.705E+01  0.123E+01  0.687E+01  0.129E+01  0.200E+01  0.818E+01  -.283E+01  0.103E+02
 36     PH                 11       4    6   0.705E+01  0.131E+01  0.686E+01  0.129E+01  0.248E+01  0.821E+01  -.240E+01  0.753E+01
 37     PH                 11       5    6   0.697E+01  0.155E+01  0.668E+01  0.141E+01  0.161E+01  0.817E+01  -.234E+01  0.718E+01
 38     PH                 11       6    6   0.679E+01  0.175E+01  0.643E+01  0.147E+01  0.161E+01  0.810E+01  -.191E+01  0.508E+01
 39     PH                 11       7    6   0.643E+01  0.199E+01  0.599E+01  0.153E+01  0.161E+01  0.814E+01  -.118E+01  0.268E+01
 40     PH                 11       8    6   0.618E+01  0.218E+01  0.564E+01  0.161E+01  0.161E+01  0.819E+01  -.964E+00  0.216E+01
 41     PH                 11       9    6   0.576E+01  0.229E+01  0.519E+01  0.164E+01  0.162E+01  0.818E+01  -.514E+00  0.147E+01
 42     PH                 11      10    6   0.553E+01  0.236E+01  0.493E+01  0.168E+01  0.161E+01  0.816E+01  -.358E+00  0.132E+01
 43     PH                 11      11    6   0.525E+01  0.246E+01  0.458E+01  0.175E+01  0.161E+01  0.815E+01  -.195E+00  0.121E+01
 44     PH                 11      12    6   0.502E+01  0.246E+01  0.435E+01  0.176E+01  0.159E+01  0.807E+01  -.392E-01  0.118E+01
 45     PH                 11      13    6   0.458E+01  0.244E+01  0.394E+01  0.176E+01  0.158E+01  0.806E+01  0.279E+00  0.126E+01
 46     PH                 11      14    6   0.453E+01  0.246E+01  0.386E+01  0.179E+01  0.107E+01  0.801E+01  0.268E+00  0.126E+01
 47     PH                 11      15    6   0.442E+01  0.243E+01  0.378E+01  0.177E+01  0.158E+01  0.794E+01  0.354E+00  0.131E+01
 48     PH                 11      16    6   0.412E+01  0.235E+01  0.352E+01  0.175E+01  0.154E+01  0.793E+01  0.592E+00  0.159E+01
```

Table D.1 continued

49	AFLUX	1	1	6	0.487E+01	0.326E+01	0.380E+01	0.215E+01	0.410E+00	0.126E+02	0.830E+00	0.273E+01
50	AFLUX	1	2	6	0.628E+01	0.300E+01	0.504E+01	0.227E+01	0.347E+00	0.122E+02	-.508E+00	0.241E+01
51	AFLUX	1	3	6	0.528E+01	0.209E+01	0.459E+01	0.194E+01	0.324E+00	0.102E+02	-.354E+00	0.319E+01
52	AFLUX	1	4	6	0.465E+01	0.165E+01	0.426E+01	0.167E+01	0.311E+00	0.104E+02	0.450E+00	0.523E+01
53	AFLUX	1	5	6	0.363E+01	0.136E+01	0.329E+01	0.168E+01	0.301E+00	0.759E+01	0.148E+00	0.356E-01
54	AFLUX	1	6	6	0.319E+01	0.106E+01	0.299E+01	0.146E+01	0.107E+01	0.532E+01	-.173E-02	0.216E+01
55	AFLUX	1	7	6	0.295E+01	0.989E+00	0.277E+01	0.145E+01	0.105E+01	0.496E+01	0.607E-01	0.225E+01
56	AFLUX	1	8	6	0.269E+01	0.951E+00	0.251E+01	0.148E+01	0.102E+01	0.468E+01	0.105E+00	0.231E+01
57	AFLUX	1	9	6	0.246E+01	0.970E+00	0.233E+01	0.151E+01	0.000E+00	0.434E+01	-.210E+00	0.247E+01
58	AFLUX	1	10	6	0.229E+01	0.915E+00	0.217E+01	0.151E+01	0.000E+00	0.410E+01	-.201E+00	0.228E+01
59	AFLUX	1	11	6	0.216E+01	0.887E+00	0.203E+01	0.151E+01	0.000E+00	0.396E+01	-.620E-01	0.219E+01
60	AFLUX	1	12	6	0.191E+01	0.913E+00	0.188E+01	0.150E+01	0.000E+00	0.381E+01	-.634E-01	0.247E+01
61	AFLUX	1	13	6	0.168E+01	0.948E+00	0.177E+01	0.149E+01	0.000E+00	0.364E+01	-.532E-01	0.241E+01
62	AFLUX	1	14	6	0.147E+01	0.942E+00	0.166E+01	0.148E+01	0.000E+00	0.351E+01	-.135E-01	0.225E+01
63	AFLUX	1	15	6	0.104E+01	0.877E+00	0.142E+01	0.154E+01	0.000E+00	0.279E+01	0.218E+00	0.198E+01
64	AFLUX	1	16	6	0.825E+00	0.783E+00	0.128E+01	0.149E+01	0.000E+00	0.269E+01	0.364E+00	0.207E+01
65	AFLUX	5	1	6	0.174E+01	0.835E+00	0.158E+01	0.158E+01	0.490E+00	0.484E+01	0.156E+01	0.642E+01
66	AFLUX	5	2	6	0.255E+01	0.179E+01	0.203E+01	0.200E+01	0.450E+00	0.794E+01	0.109E+01	0.332E+01
67	AFLUX	5	3	6	0.354E+01	0.174E+01	0.298E+01	0.196E+01	0.417E+00	0.744E+01	-.444E-02	0.240E+01
68	AFLUX	5	4	6	0.364E+01	0.158E+01	0.317E+01	0.186E+01	0.398E+00	0.659E+01	-.112E+00	0.251E+01
69	AFLUX	5	5	6	0.364E+01	0.153E+01	0.327E+01	0.168E+01	0.384E+00	0.886E+01	0.793E+00	0.479E+01
70	AFLUX	5	6	6	0.340E+01	0.130E+01	0.312E+01	0.160E+01	0.313E+00	0.760E+01	0.830E+00	0.450E+01
71	AFLUX	5	7	6	0.313E+01	0.111E+01	0.294E+01	0.143E+01	0.112E+01	0.660E+01	0.850E+00	0.392E+01
72	AFLUX	5	8	6	0.287E+01	0.106E+01	0.268E+01	0.147E+01	0.892E+00	0.562E+01	0.643E+00	0.308E+01
73	AFLUX	5	9	6	0.268E+01	0.995E+00	0.250E+01	0.148E+01	0.809E+00	0.525E+01	0.530E+00	0.296E+01
74	AFLUX	5	10	6	0.248E+01	0.879E+00	0.232E+01	0.146E+01	0.725E+00	0.437E+01	0.397E+00	0.241E+01
75	AFLUX	5	11	6	0.237E+01	0.902E+00	0.220E+01	0.149E+01	0.677E+00	0.436E+01	0.470E+00	0.235E+01
76	AFLUX	5	12	6	0.224E+01	0.869E+00	0.208E+01	0.150E+01	0.653E+00	0.431E+01	0.461E+00	0.235E+01
77	AFLUX	5	13	6	0.220E+01	0.883E+00	0.203E+01	0.151E+01	0.628E+00	0.443E+01	0.617E+00	0.261E+01
78	AFLUX	5	14	6	0.212E+01	0.913E+00	0.194E+01	0.156E+01	0.578E+00	0.428E+01	0.672E+00	0.255E+01
79	AFLUX	5	15	6	0.199E+01	0.778E+00	0.184E+01	0.151E+01	0.542E+00	0.363E+01	0.523E+00	0.245E+01
80	AFLUX	5	16	6	0.191E+01	0.727E+00	0.177E+01	0.150E+01	0.527E+00	0.336E+01	0.454E+00	0.233E+01
81	AFLUX	11	1	6	0.139E+01	0.158E+01	0.819E+00	0.287E+01	0.104E+00	0.870E+01	0.242E+01	0.106E+02
82	AFLUX	11	2	6	0.161E+02	0.122E+02	0.118E+02	0.230E+01	0.245E+01	0.465E+02	0.839E+00	0.259E+01
83	AFLUX	11	3	6	0.214E+02	0.119E+02	0.175E+02	0.205E+01	0.223E+01	0.545E+02	0.458E+00	0.280E+01
84	AFLUX	11	4	6	0.217E+02	0.103E+02	0.185E+02	0.193E+01	0.210E+01	0.481E+02	0.227E+00	0.273E+01
85	AFLUX	11	5	6	0.220E+02	0.949E+01	0.198E+02	0.168E+01	0.202E+01	0.474E+02	0.618E+00	0.307E+01
86	AFLUX	11	6	6	0.207E+02	0.900E+01	0.185E+02	0.170E+01	0.174E+01	0.431E+02	0.597E+00	0.283E+01
87	AFLUX	11	7	6	0.206E+02	0.929E+01	0.187E+02	0.154E+01	0.721E+01	0.516E+02	0.107E+01	0.401E+01
88	AFLUX	11	8	6	0.199E+02	0.950E+01	0.180E+02	0.156E+01	0.737E+01	0.548E+02	0.131E+01	0.511E+01
89	AFLUX	11	9	6	0.192E+02	0.908E+01	0.175E+02	0.153E+01	0.788E+01	0.525E+02	0.141E+01	0.529E+01
90	AFLUX	11	10	6	0.184E+02	0.859E+01	0.168E+02	0.152E+01	0.835E+01	0.519E+02	0.155E+01	0.605E+01
91	AFLUX	11	11	6	0.179E+02	0.855E+01	0.163E+02	0.153E+01	0.812E+01	0.511E+02	0.157E+01	0.604E+01
92	AFLUX	11	12	6	0.174E+02	0.835E+01	0.158E+02	0.154E+01	0.759E+01	0.455E+02	0.130E+01	0.442E+01
93	AFLUX	11	13	6	0.167E+02	0.774E+01	0.152E+02	0.154E+01	0.723E+01	0.363E+02	0.977E+00	0.294E+01
94	AFLUX	11	14	6	0.158E+02	0.783E+01	0.142E+02	0.159E+01	0.600E+01	0.353E+02	0.104E+01	0.301E+01
95	AFLUX	11	15	6	0.149E+02	0.710E+01	0.135E+02	0.155E+01	0.596E+01	0.349E+02	0.114E+01	0.347E+01
96	AFLUX	11	16	6	0.140E+02	0.678E+01	0.127E+02	0.157E+01	0.524E+01	0.345E+02	0.127E+01	0.423E+01
97	ATOTAL	1	1	6	0.100E+02	0.547E+01	0.849E+01	0.187E+01	0.163E+01	0.231E+02	0.539E+00	0.255E+01
98	ATOTAL	1	2	6	0.481E+02	0.233E+02	0.402E+02	0.200E+01	0.518E+01	0.899E+02	-.220E+00	0.201E+01
99	ATOTAL	1	3	6	0.837E+02	0.356E+02	0.726E+02	0.188E+01	0.851E+01	0.158E+03	-.361E+00	0.245E+01
100	ATOTAL	1	4	6	0.114E+03	0.411E+02	0.104E+03	0.164E+01	0.117E+02	0.203E+03	-.315E+00	0.257E+01
101	ATOTAL	1	5	6	0.139E+03	0.439E+02	0.130E+03	0.155E+01	0.149E+02	0.240E+03	-.299E+00	0.297E+01

Table D.1 continued

102	ATOTAL	1	6	6	0.160E+03	0.479E+02	0.151E+03	0.149E+01	0.216E+02	0.274E+03	-.241E+00	0.313E+01
103	ATOTAL	1	7	6	0.179E+03	0.523E+02	0.170E+03	0.144E+01	0.311E+02	0.306E+03	-.157E+00	0.308E+01
104	ATOTAL	1	8	6	0.197E+03	0.567E+02	0.188E+03	0.142E+01	0.396E+02	0.336E+03	-.104E+00	0.304E+01
105	ATOTAL	1	9	6	0.214E+03	0.601E+02	0.204E+03	0.140E+01	0.474E+02	0.347E+03	-.154E+00	0.286E+01
106	ATOTAL	1	10	6	0.229E+03	0.633E+02	0.219E+03	0.139E+01	0.546E+02	0.347E+03	-.232E+00	0.268E+01
107	ATOTAL	1	11	6	0.243E+03	0.664E+02	0.233E+03	0.138E+01	0.614E+02	0.365E+03	-.272E+00	0.259E+01
108	ATOTAL	1	12	6	0.257E+03	0.693E+02	0.246E+03	0.137E+01	0.679E+02	0.383E+03	-.283E+00	0.256E+01
109	ATOTAL	1	13	6	0.269E+03	0.713E+02	0.258E+03	0.136E+01	0.742E+02	0.401E+03	-.280E+00	0.262E+01
110	ATOTAL	1	14	6	0.279E+03	0.726E+02	0.268E+03	0.135E+01	0.801E+02	0.410E+03	-.274E+00	0.269E+01
111	ATOTAL	1	15	6	0.288E+03	0.722E+02	0.277E+03	0.134E+01	0.854E+02	0.415E+03	-.312E+00	0.281E+01
112	ATOTAL	1	16	6	0.294E+03	0.703E+02	0.284E+03	0.132E+01	0.884E+02	0.415E+03	-.414E+00	0.302E+01
113	ATOTAL	5	1	6	0.107E+02	0.343E+01	0.102E+02	0.137E+01	0.498E+01	0.217E+02	0.768E+00	0.373E+01
114	ATOTAL	5	2	6	0.106E+03	0.618E+02	0.925E+02	0.167E+01	0.230E+02	0.379E+03	0.206E+01	0.897E+01
115	ATOTAL	5	3	6	0.250E+03	0.123E+03	0.219E+03	0.174E+01	0.374E+02	0.731E+03	0.113E+01	0.608E+01
116	ATOTAL	5	4	6	0.396E+03	0.176E+03	0.352E+03	0.172E+01	0.508E+02	0.106E+04	0.862E+00	0.561E+01
117	ATOTAL	5	5	6	0.536E+03	0.201E+03	0.495E+03	0.156E+01	0.636E+02	0.131E+04	0.969E+00	0.605E+01
118	ATOTAL	5	6	6	0.663E+03	0.222E+03	0.621E+03	0.151E+01	0.764E+02	0.149E+04	0.875E+00	0.585E+01
119	ATOTAL	5	7	6	0.776E+03	0.245E+03	0.735E+03	0.143E+01	0.134E+03	0.167E+04	0.858E+00	0.549E+01
120	ATOTAL	5	8	6	0.878E+03	0.266E+03	0.837E+03	0.139E+01	0.199E+03	0.184E+04	0.875E+00	0.529E+01
121	ATOTAL	5	9	6	0.972E+03	0.288E+03	0.930E+03	0.137E+01	0.258E+03	0.201E+04	0.894E+00	0.513E+01
122	ATOTAL	5	10	6	0.106E+04	0.311E+03	0.102E+04	0.135E+01	0.312E+03	0.217E+04	0.915E+00	0.504E+01
123	ATOTAL	5	11	6	0.114E+04	0.333E+03	0.110E+04	0.134E+01	0.362E+03	0.233E+04	0.941E+00	0.501E+01
124	ATOTAL	5	12	6	0.122E+04	0.355E+03	0.117E+04	0.134E+01	0.412E+03	0.249E+04	0.957E+00	0.494E+01
125	ATOTAL	5	13	6	0.130E+04	0.377E+03	0.125E+04	0.134E+01	0.459E+03	0.264E+04	0.975E+00	0.492E+01
126	ATOTAL	5	14	6	0.137E+04	0.396E+03	0.132E+04	0.133E+01	0.505E+03	0.279E+04	0.989E+00	0.496E+01
127	ATOTAL	5	15	6	0.144E+04	0.413E+03	0.138E+04	0.133E+01	0.547E+03	0.294E+04	0.101E+01	0.507E+01
128	ATOTAL	5	16	6	0.150E+04	0.429E+03	0.144E+04	0.133E+01	0.576E+03	0.307E+04	0.101E+01	0.518E+01
129	ATOTAL	11	1	6	0.715E+01	0.734E+01	0.425E+01	0.282E+01	0.764E+00	0.255E+02	0.114E+01	0.293E+01
130	ATOTAL	11	2	6	0.138E+03	0.720E+02	0.122E+03	0.162E+01	0.424E+02	0.352E+03	0.121E+01	0.397E+01
131	ATOTAL	11	3	6	0.351E+03	0.167E+03	0.311E+03	0.167E+01	0.746E+02	0.800E+03	0.654E+00	0.301E+01
132	ATOTAL	11	4	6	0.588E+03	0.257E+03	0.527E+03	0.166E+01	0.105E+03	0.124E+04	0.443E+00	0.292E+01
133	ATOTAL	11	5	6	0.826E+03	0.319E+03	0.760E+03	0.156E+01	0.133E+03	0.160E+04	0.464E+00	0.301E+01
134	ATOTAL	11	6	6	0.106E+04	0.371E+03	0.985E+03	0.151E+01	0.160E+03	0.197E+04	0.461E+00	0.319E+01
135	ATOTAL	11	7	6	0.128E+04	0.418E+03	0.120E+04	0.145E+01	0.246E+03	0.235E+04	0.486E+00	0.332E+01
136	ATOTAL	11	8	6	0.149E+04	0.460E+03	0.142E+04	0.139E+01	0.399E+03	0.265E+04	0.532E+00	0.322E+01
137	ATOTAL	11	9	6	0.169E+04	0.499E+03	0.162E+04	0.136E+01	0.548E+03	0.294E+04	0.559E+00	0.314E+01
138	ATOTAL	11	10	6	0.189E+04	0.537E+03	0.181E+04	0.134E+01	0.686E+03	0.322E+04	0.579E+00	0.309E+01
139	ATOTAL	11	11	6	0.207E+04	0.574E+03	0.200E+04	0.132E+01	0.816E+03	0.349E+04	0.602E+00	0.305E+01
140	ATOTAL	11	12	6	0.226E+04	0.614E+03	0.218E+04	0.131E+01	0.933E+03	0.376E+04	0.608E+00	0.300E+01
141	ATOTAL	11	13	6	0.243E+04	0.652E+03	0.235E+04	0.131E+01	0.104E+04	0.402E+04	0.602E+00	0.296E+01
142	ATOTAL	11	14	6	0.260E+04	0.687E+03	0.251E+04	0.130E+01	0.114E+04	0.423E+04	0.579E+00	0.290E+01
143	ATOTAL	11	15	6	0.276E+04	0.718E+03	0.267E+04	0.130E+01	0.124E+04	0.442E+04	0.567E+00	0.286E+01
144	ATOTAL	11	16	6	0.292E+04	0.749E+03	0.282E+04	0.129E+01	0.131E+04	0.461E+04	0.539E+00	0.282E+01
145	AYEAR	1	1	6	0.100E+02	0.547E+01	0.849E+01	0.187E+01	0.163E+01	0.231E+02	0.539E+00	0.255E+01
146	AYEAR	1	2	6	0.122E+02	0.568E+01	0.102E+02	0.200E+01	0.142E+01	0.248E+02	-.322E+00	0.239E+01
147	AYEAR	1	3	6	0.100E+02	0.387E+01	0.902E+01	0.172E+01	0.137E+01	0.201E+02	-.152E+00	0.311E+01
148	AYEAR	1	4	6	0.876E+01	0.317E+01	0.812E+01	0.154E+01	0.134E+01	0.204E+02	0.802E+00	0.564E+01
149	AYEAR	1	5	6	0.693E+01	0.247E+01	0.645E+01	0.151E+01	0.132E+01	0.141E+02	0.434E+00	0.345E+01
150	AYEAR	1	6	6	0.618E+01	0.192E+01	0.587E+01	0.139E+01	0.252E+01	0.109E+02	0.317E+00	0.256E+01
151	AYEAR	1	7	6	0.576E+01	0.177E+01	0.549E+01	0.138E+01	0.246E+01	0.102E+02	0.357E+00	0.272E+01
152	AYEAR	1	8	6	0.536E+01	0.165E+01	0.511E+01	0.138E+01	0.220E+01	0.950E+01	0.445E+00	0.289E+01
153	AYEAR	1	9	6	0.491E+01	0.162E+01	0.478E+01	0.138E+01	-.531E-01	0.809E+01	-.423E+00	0.347E+01
154	AYEAR	1	10	6	0.463E+01	0.151E+01	0.451E+01	0.137E+01	-.531E-01	0.760E+01	-.481E+00	0.342E+01

Table D.1 continued

155	AYEAR	1	11	6	0.441E+01	0.148E+01	0.428E+01	0.139E+01	-.531E-01	0.734E+01	-.397E+00	0.316E+01
156	AYEAR	1	12	6	0.397E+01	0.160E+01	0.403E+01	0.138E+01	-.531E-01	0.703E+01	-.604E+00	0.343E+01
157	AYEAR	1	13	6	0.351E+01	0.174E+01	0.381E+01	0.137E+01	-.689E-01	0.670E+01	-.588E+00	0.295E+01
158	AYEAR	1	14	6	0.312E+01	0.176E+01	0.353E+01	0.141E+01	-.689E-01	0.658E+01	-.488E+00	0.250E+01
159	AYEAR	1	15	6	0.227E+01	0.178E+01	0.322E+01	0.177E+01	-.689E-01	0.508E+01	-.224E+00	0.164E+01
160	AYEAR	1	16	6	0.186E+01	0.169E+01	0.299E+01	0.139E+01	-.689E-01	0.481E+01	-.145E-01	0.144E+01
161	AYEAR	5	1	6	0.107E+02	0.343E+01	0.102E+02	0.137E+01	0.498E+01	0.217E+02	0.768E+00	0.373E+01
162	AYEAR	5	2	6	0.164E+02	0.105E+02	0.140E+02	0.172E+01	0.641E+01	0.423E+02	0.130E+01	0.328E+01
163	AYEAR	5	3	6	0.249E+02	0.118E+02	0.217E+02	0.177E+01	0.591E+01	0.480E+02	0.237E-01	0.182E+01
164	AYEAR	5	4	6	0.248E+02	0.108E+02	0.225E+02	0.160E+01	0.561E+01	0.634E+02	0.987E+00	0.497E+01
165	AYEAR	5	5	6	0.254E+02	0.127E+02	0.230E+02	0.156E+01	0.541E+01	0.784E+02	0.203E+01	0.832E+01
166	AYEAR	5	6	6	0.232E+02	0.106E+02	0.213E+02	0.151E+01	0.567E+01	0.626E+02	0.186E+01	0.724E+01
167	AYEAR	5	7	6	0.212E+02	0.851E+01	0.198E+02	0.144E+01	0.656E+01	0.545E+02	0.164E+01	0.668E+01
168	AYEAR	5	8	6	0.189E+02	0.682E+01	0.177E+02	0.142E+01	0.689E+01	0.394E+02	0.888E+00	0.354E+01
169	AYEAR	5	9	6	0.177E+02	0.633E+01	0.167E+02	0.142E+01	0.677E+01	0.330E+02	0.689E+00	0.265E+01
170	AYEAR	5	10	6	0.168E+02	0.606E+01	0.158E+02	0.142E+01	0.669E+01	0.336E+02	0.832E+00	0.302E+01
171	AYEAR	5	11	6	0.162E+02	0.589E+01	0.153E+02	0.142E+01	0.660E+01	0.317E+02	0.819E+00	0.288E+01
172	AYEAR	5	12	6	0.158E+02	0.590E+01	0.148E+02	0.143E+01	0.650E+01	0.314E+02	0.907E+00	0.323E+01
173	AYEAR	5	13	6	0.153E+02	0.574E+01	0.143E+02	0.143E+01	0.644E+01	0.317E+02	0.959E+00	0.362E+01
174	AYEAR	5	14	6	0.149E+02	0.558E+01	0.140E+02	0.143E+01	0.638E+01	0.313E+02	0.997E+00	0.384E+01
175	AYEAR	5	15	6	0.142E+02	0.492E+01	0.134E+02	0.140E+01	0.629E+01	0.288E+02	0.896E+00	0.347E+01
176	AYEAR	5	16	6	0.138E+02	0.495E+01	0.130E+02	0.140E+01	0.621E+01	0.289E+02	0.117E+01	0.436E+01
177	AYEAR	11	1	6	0.715E+01	0.734E+01	0.425E+01	0.282E+01	0.764E+00	0.255E+02	0.114E+01	0.293E+01
178	AYEAR	11	2	6	0.117E+03	0.779E+02	0.951E+02	0.192E+01	0.249E+02	0.342E+03	0.113E+01	0.369E+01
179	AYEAR	11	3	6	0.171E+03	0.908E+02	0.143E+03	0.198E+01	0.223E+02	0.367E+03	0.294E+00	0.239E+01
180	AYEAR	11	4	6	0.176E+03	0.837E+02	0.153E+03	0.183E+01	0.209E+02	0.383E+03	0.409E+00	0.280E+01
181	AYEAR	11	5	6	0.173E+03	0.649E+02	0.159E+03	0.157E+01	0.200E+02	0.333E+03	0.536E+00	0.326E+01
182	AYEAR	11	6	6	0.163E+03	0.599E+02	0.150E+03	0.157E+01	0.183E+02	0.311E+03	0.439E+00	0.317E+01
183	AYEAR	11	7	6	0.153E+03	0.519E+02	0.145E+03	0.140E+01	0.695E+02	0.305E+03	0.774E+00	0.359E+01
184	AYEAR	11	8	6	0.148E+03	0.482E+02	0.141E+03	0.138E+01	0.722E+02	0.280E+03	0.685E+00	0.305E+01
185	AYEAR	11	9	6	0.141E+03	0.430E+02	0.135E+03	0.136E+01	0.686E+02	0.241E+03	0.539E+00	0.261E+01
186	AYEAR	11	10	6	0.136E+03	0.418E+02	0.130E+03	0.136E+01	0.683E+02	0.236E+03	0.545E+00	0.266E+01
187	AYEAR	11	11	6	0.131E+03	0.417E+02	0.124E+03	0.138E+01	0.651E+02	0.228E+03	0.559E+00	0.252E+01
188	AYEAR	11	12	6	0.128E+03	0.413E+02	0.121E+03	0.138E+01	0.639E+02	0.222E+03	0.547E+00	0.248E+01
189	AYEAR	11	13	6	0.123E+03	0.394E+02	0.117E+03	0.139E+01	0.535E+02	0.209E+03	0.407E+00	0.236E+01
190	AYEAR	11	14	6	0.117E+03	0.355E+02	0.112E+03	0.137E+01	0.575E+02	0.202E+03	0.348E+00	0.242E+01
191	AYEAR	11	15	6	0.113E+03	0.340E+02	0.107E+03	0.137E+01	0.517E+02	0.198E+03	0.376E+00	0.268E+01
192	AYEAR	11	16	6	0.105E+03	0.319E+02	0.998E+02	0.137E+01	0.505E+02	0.188E+03	0.386E+00	0.268E+01

```
Table D.2  KEY.NOM

FILE CREATED 03/19/87 AT 09:29:17
 DETERMINISTIC ANALYSIS: INPUTD.DAT
 NUMBER OF TRIALS:     1
     PARAMETER          LOCATION  YEAR MONTH    MEAN     STD DEV   GEOM MEAN   GEOM SD    MINIMUM    MAXIMUM
   1    PH                  1       1    6   0.676E+01            0.676E+01              0.676E+01  0.676E+01
   2    PH                  1       2    6   0.674E+01            0.674E+01              0.674E+01  0.674E+01
   3    PH                  1       3    6   0.364E+01            0.364E+01              0.364E+01  0.364E+01
   4    PH                  1       4    6   0.367E+01            0.367E+01              0.367E+01  0.367E+01
   5    PH                  1       5    6   0.369E+01            0.369E+01              0.369E+01  0.369E+01
   6    PH                  1       6    6   0.205E+01            0.205E+01              0.205E+01  0.205E+01
   7    PH                  1       7    6   0.206E+01            0.206E+01              0.206E+01  0.206E+01
   8    PH                  1       8    6   0.207E+01            0.207E+01              0.207E+01  0.207E+01
   9    PH                  1       9    6   0.207E+01            0.207E+01              0.207E+01  0.207E+01
  10    PH                  1      10    6   0.208E+01            0.208E+01              0.208E+01  0.208E+01
  11    PH                  1      11    6   0.209E+01            0.209E+01              0.209E+01  0.209E+01
  12    PH                  1      12    6   0.210E+01            0.210E+01              0.210E+01  0.210E+01
  13    PH                  1      13    6   0.213E+01            0.213E+01              0.213E+01  0.213E+01
  14    PH                  1      14    6   0.227E+01            0.227E+01              0.227E+01  0.227E+01
  15    PH                  1      15    6   0.228E+01            0.228E+01              0.228E+01  0.228E+01
  16    PH                  1      16    6   0.228E+01            0.228E+01              0.228E+01  0.228E+01
  17    PH                  1      17    6   0.228E+01            0.228E+01              0.228E+01  0.228E+01
  18    PH                  1      18    6   0.228E+01            0.228E+01              0.228E+01  0.228E+01
  19    PH                  1      19    6   0.229E+01            0.229E+01              0.229E+01  0.229E+01
  20    PH                  1      20    6   0.229E+01            0.229E+01              0.229E+01  0.229E+01
  21    PH                  1      21    6   0.218E+01            0.218E+01              0.218E+01  0.218E+01
  22    PH                  5       1    6   0.682E+01            0.682E+01              0.682E+01  0.682E+01
  23    PH                  5       2    6   0.678E+01            0.678E+01              0.678E+01  0.678E+01
  24    PH                  5       3    6   0.365E+01            0.365E+01              0.365E+01  0.365E+01
  25    PH                  5       4    6   0.366E+01            0.366E+01              0.366E+01  0.366E+01
  26    PH                  5       5    6   0.369E+01            0.369E+01              0.369E+01  0.369E+01
  27    PH                  5       6    6   0.370E+01            0.370E+01              0.370E+01  0.370E+01
  28    PH                  5       7    6   0.201E+01            0.201E+01              0.201E+01  0.201E+01
  29    PH                  5       8    6   0.201E+01            0.201E+01              0.201E+01  0.201E+01
  30    PH                  5       9    6   0.201E+01            0.201E+01              0.201E+01  0.201E+01
  31    PH                  5      10    6   0.202E+01            0.202E+01              0.202E+01  0.202E+01
  32    PH                  5      11    6   0.203E+01            0.203E+01              0.203E+01  0.203E+01
  33    PH                  5      12    6   0.203E+01            0.203E+01              0.203E+01  0.203E+01
  34    PH                  5      13    6   0.205E+01            0.205E+01              0.205E+01  0.205E+01
  35    PH                  5      14    6   0.205E+01            0.205E+01              0.205E+01  0.205E+01
  36    PH                  5      15    6   0.206E+01            0.206E+01              0.206E+01  0.206E+01
  37    PH                  5      16    6   0.206E+01            0.206E+01              0.206E+01  0.206E+01
  38    PH                  5      17    6   0.206E+01            0.206E+01              0.206E+01  0.206E+01
  39    PH                  5      18    6   0.207E+01            0.207E+01              0.207E+01  0.207E+01
  40    PH                  5      19    6   0.207E+01            0.207E+01              0.207E+01  0.207E+01
  41    PH                  5      20    6   0.208E+01            0.208E+01              0.208E+01  0.208E+01
  42    PH                  5      21    6   0.209E+01            0.209E+01              0.209E+01  0.209E+01
  43    PH                 11       1    6   0.691E+01            0.691E+01              0.691E+01  0.691E+01
  44    PH                 11       2    6   0.698E+01            0.698E+01              0.698E+01  0.698E+01
  45    PH                 11       3    6   0.727E+01            0.727E+01              0.727E+01  0.727E+01
  46    PH                 11       4    6   0.273E+01            0.273E+01              0.273E+01  0.273E+01
  47    PH                 11       5    6   0.222E+01            0.222E+01              0.222E+01  0.222E+01
  48    PH                 11       6    6   0.222E+01            0.222E+01              0.222E+01  0.222E+01
  49    PH                 11       7    6   0.224E+01            0.224E+01              0.224E+01  0.224E+01
```

Table D.2 continued

50	PH	11	8	6	0.224E+01	0.224E+01	0.224E+01	0.224E+01
51	PH	11	9	6	0.220E+01	0.220E+01	0.220E+01	0.220E+01
52	PH	11	10	6	0.220E+01	0.220E+01	0.220E+01	0.220E+01
53	PH	11	11	6	0.220E+01	0.220E+01	0.220E+01	0.220E+01
54	PH	11	12	6	0.220E+01	0.220E+01	0.220E+01	0.220E+01
55	PH	11	13	6	0.220E+01	0.220E+01	0.220E+01	0.220E+01
56	PH	11	14	6	0.220E+01	0.220E+01	0.220E+01	0.220E+01
57	PH	11	15	6	0.220E+01	0.220E+01	0.220E+01	0.220E+01
58	PH	11	16	6	0.220E+01	0.220E+01	0.220E+01	0.220E+01
59	PH	11	17	6	0.220E+01	0.220E+01	0.220E+01	0.220E+01
60	PH	11	18	6	0.220E+01	0.220E+01	0.220E+01	0.220E+01
61	PH	11	19	6	0.220E+01	0.220E+01	0.220E+01	0.220E+01
62	PH	11	20	6	0.220E+01	0.220E+01	0.220E+01	0.220E+01
63	PH	11	21	6	0.220E+01	0.220E+01	0.220E+01	0.220E+01
64	AFLUX	1	1	6	0.686E+00	0.686E+00	0.686E+00	0.686E+00
65	AFLUX	1	2	6	0.566E+00	0.566E+00	0.566E+00	0.566E+00
66	AFLUX	1	3	6	0.283E+01	0.283E+01	0.283E+01	0.283E+01
67	AFLUX	1	4	6	0.234E+01	0.234E+01	0.234E+01	0.234E+01
68	AFLUX	1	5	6	0.208E+01	0.208E+01	0.208E+01	0.208E+01
69	AFLUX	1	6	6	0.690E+00	0.690E+00	0.690E+00	0.690E+00
70	AFLUX	1	7	6	0.670E+00	0.670E+00	0.670E+00	0.670E+00
71	AFLUX	1	8	6	0.648E+00	0.648E+00	0.648E+00	0.648E+00
72	AFLUX	1	9	6	0.630E+00	0.630E+00	0.630E+00	0.630E+00
73	AFLUX	1	10	6	0.611E+00	0.611E+00	0.611E+00	0.611E+00
74	AFLUX	1	11	6	0.596E+00	0.596E+00	0.596E+00	0.596E+00
75	AFLUX	1	12	6	0.582E+00	0.582E+00	0.582E+00	0.582E+00
76	AFLUX	1	13	6	0.524E+00	0.524E+00	0.524E+00	0.524E+00
77	AFLUX	1	14	6	0.131E+01	0.131E+01	0.131E+01	0.131E+01
78	AFLUX	1	15	6	0.129E+01	0.129E+01	0.129E+01	0.129E+01
79	AFLUX	1	16	6	0.127E+01	0.127E+01	0.127E+01	0.127E+01
80	AFLUX	1	17	6	0.125E+01	0.125E+01	0.125E+01	0.125E+01
81	AFLUX	1	18	6	0.123E+01	0.123E+01	0.123E+01	0.123E+01
82	AFLUX	1	19	6	0.121E+01	0.121E+01	0.121E+01	0.121E+01
83	AFLUX	1	20	6	0.118E+01	0.118E+01	0.118E+01	0.118E+01
84	AFLUX	1	21	6	0.441E+00	0.441E+00	0.441E+00	0.441E+00
85	AFLUX	5	1	6	0.111E+01	0.111E+01	0.111E+01	0.111E+01
86	AFLUX	5	2	6	0.849E+00	0.849E+00	0.849E+00	0.849E+00
87	AFLUX	5	3	6	0.303E+01	0.303E+01	0.303E+01	0.303E+01
88	AFLUX	5	4	6	0.210E+01	0.210E+01	0.210E+01	0.210E+01
89	AFLUX	5	5	6	0.176E+01	0.176E+01	0.176E+01	0.176E+01
90	AFLUX	5	6	6	0.159E+01	0.159E+01	0.159E+01	0.159E+01
91	AFLUX	5	7	6	0.872E+00	0.872E+00	0.872E+00	0.872E+00
92	AFLUX	5	8	6	0.856E+00	0.856E+00	0.856E+00	0.856E+00
93	AFLUX	5	9	6	0.853E+00	0.853E+00	0.853E+00	0.853E+00
94	AFLUX	5	10	6	0.827E+00	0.827E+00	0.827E+00	0.827E+00
95	AFLUX	5	11	6	0.807E+00	0.807E+00	0.807E+00	0.807E+00
96	AFLUX	5	12	6	0.789E+00	0.789E+00	0.789E+00	0.789E+00
97	AFLUX	5	13	6	0.719E+00	0.719E+00	0.719E+00	0.719E+00
98	AFLUX	5	14	6	0.708E+00	0.708E+00	0.708E+00	0.708E+00
99	AFLUX	5	15	6	0.694E+00	0.694E+00	0.694E+00	0.694E+00
100	AFLUX	5	16	6	0.681E+00	0.681E+00	0.681E+00	0.681E+00
101	AFLUX	5	17	6	0.669E+00	0.669E+00	0.669E+00	0.669E+00
102	AFLUX	5	18	6	0.658E+00	0.658E+00	0.658E+00	0.658E+00

Table D.2 continued

103	AFLUX	5	19	6	0.648E+00	0.648E+00	0.648E+00	0.648E+00
104	AFLUX	5	20	6	0.627E+00	0.627E+00	0.627E+00	0.627E+00
105	AFLUX	5	21	6	0.599E+00	0.599E+00	0.599E+00	0.599E+00
106	AFLUX	11	1	6	0.188E+01	0.188E+01	0.188E+01	0.188E+01
107	AFLUX	11	2	6	0.267E+01	0.267E+01	0.267E+01	0.267E+01
108	AFLUX	11	3	6	0.101E+02	0.101E+02	0.101E+02	0.101E+02
109	AFLUX	11	4	6	0.177E+02	0.177E+02	0.177E+02	0.177E+02
110	AFLUX	11	5	6	0.134E+02	0.134E+02	0.134E+02	0.134E+02
111	AFLUX	11	6	6	0.124E+02	0.124E+02	0.124E+02	0.124E+02
112	AFLUX	11	7	6	0.755E+01	0.755E+01	0.755E+01	0.755E+01
113	AFLUX	11	8	6	0.639E+01	0.639E+01	0.639E+01	0.639E+01
114	AFLUX	11	9	6	0.450E+01	0.450E+01	0.450E+01	0.450E+01
115	AFLUX	11	10	6	0.429E+01	0.429E+01	0.429E+01	0.429E+01
116	AFLUX	11	11	6	0.418E+01	0.418E+01	0.418E+01	0.418E+01
117	AFLUX	11	12	6	0.409E+01	0.409E+01	0.409E+01	0.409E+01
118	AFLUX	11	13	6	0.386E+01	0.386E+01	0.386E+01	0.386E+01
119	AFLUX	11	14	6	0.379E+01	0.379E+01	0.379E+01	0.379E+01
120	AFLUX	11	15	6	0.374E+01	0.374E+01	0.374E+01	0.374E+01
121	AFLUX	11	16	6	0.368E+01	0.368E+01	0.368E+01	0.368E+01
122	AFLUX	11	17	6	0.361E+01	0.361E+01	0.361E+01	0.361E+01
123	AFLUX	11	18	6	0.355E+01	0.355E+01	0.355E+01	0.355E+01
124	AFLUX	11	19	6	0.349E+01	0.349E+01	0.349E+01	0.349E+01
125	AFLUX	11	20	6	0.338E+01	0.338E+01	0.338E+01	0.338E+01
126	AFLUX	11	21	6	0.320E+01	0.320E+01	0.320E+01	0.320E+01
127	ATOTAL	1	1	6	0.205E+01	0.205E+01	0.205E+01	0.205E+01
128	ATOTAL	1	2	6	0.646E+01	0.646E+01	0.646E+01	0.646E+01
129	ATOTAL	1	3	6	0.211E+02	0.211E+02	0.211E+02	0.211E+02
130	ATOTAL	1	4	6	0.352E+02	0.352E+02	0.352E+02	0.352E+02
131	ATOTAL	1	5	6	0.475E+02	0.475E+02	0.475E+02	0.475E+02
132	ATOTAL	1	6	6	0.573E+02	0.573E+02	0.573E+02	0.573E+02
133	ATOTAL	1	7	6	0.634E+02	0.634E+02	0.634E+02	0.634E+02
134	ATOTAL	1	8	6	0.694E+02	0.694E+02	0.694E+02	0.694E+02
135	ATOTAL	1	9	6	0.751E+02	0.751E+02	0.751E+02	0.751E+02
136	ATOTAL	1	10	6	0.807E+02	0.807E+02	0.807E+02	0.807E+02
137	ATOTAL	1	11	6	0.860E+02	0.860E+02	0.860E+02	0.860E+02
138	ATOTAL	1	12	6	0.913E+02	0.913E+02	0.913E+02	0.913E+02
139	ATOTAL	1	13	6	0.962E+02	0.962E+02	0.962E+02	0.962E+02
140	ATOTAL	1	14	6	0.102E+03	0.102E+03	0.102E+03	0.102E+03
141	ATOTAL	1	15	6	0.108E+03	0.108E+03	0.108E+03	0.108E+03
142	ATOTAL	1	16	6	0.114E+03	0.114E+03	0.114E+03	0.114E+03
143	ATOTAL	1	17	6	0.119E+03	0.119E+03	0.119E+03	0.119E+03
144	ATOTAL	1	18	6	0.125E+03	0.125E+03	0.125E+03	0.125E+03
145	ATOTAL	1	19	6	0.130E+03	0.130E+03	0.130E+03	0.130E+03
146	ATOTAL	1	20	6	0.135E+03	0.135E+03	0.135E+03	0.135E+03
147	ATOTAL	1	21	6	0.139E+03	0.139E+03	0.139E+03	0.139E+03
148	ATOTAL	5	1	6	0.791E+01	0.791E+01	0.791E+01	0.791E+01
149	ATOTAL	5	2	6	0.274E+02	0.274E+02	0.274E+02	0.274E+02
150	ATOTAL	5	3	6	0.489E+02	0.489E+02	0.489E+02	0.489E+02
151	ATOTAL	5	4	6	0.129E+03	0.129E+03	0.129E+03	0.129E+03
152	ATOTAL	5	5	6	0.194E+03	0.194E+03	0.194E+03	0.194E+03
153	ATOTAL	5	6	6	0.252E+03	0.252E+03	0.252E+03	0.252E+03
154	ATOTAL	5	7	6	0.300E+03	0.300E+03	0.300E+03	0.300E+03
155	ATOTAL	5	8	6	0.328E+03	0.328E+03	0.328E+03	0.328E+03

Table D.2 continued

156	ATOTAL	5	9	6	0.355E+03	0.355E+03	0.355E+03	0.355E+03
157	ATOTAL	5	10	6	0.382E+03	0.382E+03	0.382E+03	0.382E+03
158	ATOTAL	5	11	6	0.408E+03	0.408E+03	0.408E+03	0.408E+03
159	ATOTAL	5	12	6	0.433E+03	0.433E+03	0.433E+03	0.433E+03
160	ATOTAL	5	13	6	0.457E+03	0.457E+03	0.457E+03	0.457E+03
161	ATOTAL	5	14	6	0.479E+03	0.479E+03	0.479E+03	0.479E+03
162	ATOTAL	5	15	6	0.504E+03	0.504E+03	0.504E+03	0.504E+03
163	ATOTAL	5	16	6	0.527E+03	0.527E+03	0.527E+03	0.527E+03
164	ATOTAL	5	17	6	0.550E+03	0.550E+03	0.550E+03	0.550E+03
165	ATOTAL	5	18	6	0.573E+03	0.573E+03	0.573E+03	0.573E+03
166	ATOTAL	5	19	6	0.595E+03	0.595E+03	0.595E+03	0.595E+03
167	ATOTAL	5	20	6	0.616E+03	0.616E+03	0.616E+03	0.616E+03
168	ATOTAL	5	21	6	0.636E+03	0.636E+03	0.636E+03	0.636E+03
169	ATOTAL	11	1	6	0.127E+02	0.127E+02	0.127E+02	0.127E+02
170	ATOTAL	11	2	6	0.536E+02	0.536E+02	0.536E+02	0.536E+02
171	ATOTAL	11	3	6	0.935E+02	0.935E+02	0.935E+02	0.935E+02
172	ATOTAL	11	4	6	0.290E+03	0.290E+03	0.290E+03	0.290E+03
173	ATOTAL	11	5	6	0.465E+03	0.465E+03	0.465E+03	0.465E+03
174	ATOTAL	11	6	6	0.611E+03	0.611E+03	0.611E+03	0.611E+03
175	ATOTAL	11	7	6	0.735E+03	0.735E+03	0.735E+03	0.735E+03
176	ATOTAL	11	8	6	0.830E+03	0.830E+03	0.830E+03	0.830E+03
177	ATOTAL	11	9	6	0.904E+03	0.904E+03	0.904E+03	0.904E+03
178	ATOTAL	11	10	6	0.971E+03	0.971E+03	0.971E+03	0.971E+03
179	ATOTAL	11	11	6	0.103E+04	0.103E+04	0.103E+04	0.103E+04
180	ATOTAL	11	12	6	0.110E+04	0.110E+04	0.110E+04	0.110E+04
181	ATOTAL	11	13	6	0.116E+04	0.116E+04	0.116E+04	0.116E+04
182	ATOTAL	11	14	6	0.121E+04	0.121E+04	0.121E+04	0.121E+04
183	ATOTAL	11	15	6	0.127E+04	0.127E+04	0.127E+04	0.127E+04
184	ATOTAL	11	16	6	0.133E+04	0.133E+04	0.133E+04	0.133E+04
185	ATOTAL	11	17	6	0.138E+04	0.138E+04	0.138E+04	0.138E+04
186	ATOTAL	11	18	6	0.144E+04	0.144E+04	0.144E+04	0.144E+04
187	ATOTAL	11	19	6	0.149E+04	0.149E+04	0.149E+04	0.149E+04
188	ATOTAL	11	20	6	0.154E+04	0.154E+04	0.154E+04	0.154E+04
189	ATOTAL	11	21	6	0.159E+04	0.159E+04	0.159E+04	0.159E+04
190	AYEAR	1	1	6	0.205E+01	0.205E+01	0.205E+01	0.205E+01
191	AYEAR	1	2	6	0.168E+01	0.168E+01	0.168E+01	0.168E+01
192	AYEAR	1	3	6	0.509E+01	0.509E+01	0.509E+01	0.509E+01
193	AYEAR	1	4	6	0.410E+01	0.410E+01	0.410E+01	0.410E+01
194	AYEAR	1	5	6	0.360E+01	0.360E+01	0.360E+01	0.360E+01
195	AYEAR	1	6	6	0.202E+01	0.202E+01	0.202E+01	0.202E+01
196	AYEAR	1	7	6	0.209E+01	0.209E+01	0.209E+01	0.209E+01
197	AYEAR	1	8	6	0.203E+01	0.203E+01	0.203E+01	0.203E+01
198	AYEAR	1	9	6	0.197E+01	0.197E+01	0.197E+01	0.197E+01
199	AYEAR	1	10	6	0.190E+01	0.190E+01	0.190E+01	0.190E+01
200	AYEAR	1	11	6	0.185E+01	0.185E+01	0.185E+01	0.185E+01
201	AYEAR	1	12	6	0.180E+01	0.180E+01	0.180E+01	0.180E+01
202	AYEAR	1	13	6	0.166E+01	0.166E+01	0.166E+01	0.166E+01
203	AYEAR	1	14	6	0.329E+01	0.329E+01	0.329E+01	0.329E+01
204	AYEAR	1	15	6	0.216E+01	0.216E+01	0.216E+01	0.216E+01
205	AYEAR	1	16	6	0.212E+01	0.212E+01	0.212E+01	0.212E+01
206	AYEAR	1	17	6	0.208E+01	0.208E+01	0.208E+01	0.208E+01
207	AYEAR	1	18	6	0.205E+01	0.205E+01	0.205E+01	0.205E+01
208	AYEAR	1	19	6	0.202E+01	0.202E+01	0.202E+01	0.202E+01

Table D.2 continued

209	AYEAR	1	20	6	0.196E+01	0.196E+01	0.196E+01	0.196E+01
210	AYEAR	1	21	6	0.176E+01	0.176E+01	0.176E+01	0.176E+01
211	AYEAR	5	1	6	0.791E+01	0.791E+01	0.791E+01	0.791E+01
212	AYEAR	5	2	6	0.574E+01	0.574E+01	0.574E+01	0.574E+01
213	AYEAR	5	3	6	0.105E+02	0.105E+02	0.105E+02	0.105E+02
214	AYEAR	5	4	6	0.624E+01	0.624E+01	0.624E+01	0.624E+01
215	AYEAR	5	5	6	0.497E+01	0.497E+01	0.497E+01	0.497E+01
216	AYEAR	5	6	6	0.455E+01	0.455E+01	0.455E+01	0.455E+01
217	AYEAR	5	7	6	0.328E+01	0.328E+01	0.328E+01	0.328E+01
218	AYEAR	5	8	6	0.325E+01	0.325E+01	0.325E+01	0.325E+01
219	AYEAR	5	9	6	0.349E+01	0.349E+01	0.349E+01	0.349E+01
220	AYEAR	5	10	6	0.324E+01	0.324E+01	0.324E+01	0.324E+01
221	AYEAR	5	11	6	0.317E+01	0.317E+01	0.317E+01	0.317E+01
222	AYEAR	5	12	6	0.314E+01	0.314E+01	0.314E+01	0.314E+01
223	AYEAR	5	13	6	0.274E+01	0.274E+01	0.274E+01	0.274E+01
224	AYEAR	5	14	6	0.270E+01	0.270E+01	0.270E+01	0.270E+01
225	AYEAR	5	15	6	0.273E+01	0.273E+01	0.273E+01	0.273E+01
226	AYEAR	5	16	6	0.269E+01	0.269E+01	0.269E+01	0.269E+01
227	AYEAR	5	17	6	0.264E+01	0.264E+01	0.264E+01	0.264E+01
228	AYEAR	5	18	6	0.260E+01	0.260E+01	0.260E+01	0.260E+01
229	AYEAR	5	19	6	0.244E+01	0.244E+01	0.244E+01	0.244E+01
230	AYEAR	5	20	6	0.237E+01	0.237E+01	0.237E+01	0.237E+01
231	AYEAR	5	21	6	0.220E+01	0.220E+01	0.220E+01	0.220E+01
232	AYEAR	11	1	6	0.127E+02	0.127E+02	0.127E+02	0.127E+02
233	AYEAR	11	2	6	0.254E+02	0.254E+02	0.254E+02	0.254E+02
234	AYEAR	11	3	6	0.270E+02	0.270E+02	0.270E+02	0.270E+02
235	AYEAR	11	4	6	0.169E+03	0.169E+03	0.169E+03	0.169E+03
236	AYEAR	11	5	6	0.125E+03	0.125E+03	0.125E+03	0.125E+03
237	AYEAR	11	6	6	0.107E+03	0.107E+03	0.107E+03	0.107E+03
238	AYEAR	11	7	6	0.886E+02	0.886E+02	0.886E+02	0.886E+02
239	AYEAR	11	8	6	0.631E+02	0.631E+02	0.631E+02	0.631E+02
240	AYEAR	11	9	6	0.462E+02	0.462E+02	0.462E+02	0.462E+02
241	AYEAR	11	10	6	0.441E+02	0.441E+02	0.441E+02	0.441E+02
242	AYEAR	11	11	6	0.429E+02	0.429E+02	0.429E+02	0.429E+02
243	AYEAR	11	12	6	0.418E+02	0.418E+02	0.418E+02	0.418E+02
244	AYEAR	11	13	6	0.398E+02	0.398E+02	0.398E+02	0.398E+02
245	AYEAR	11	14	6	0.368E+02	0.368E+02	0.368E+02	0.368E+02
246	AYEAR	11	15	6	0.406E+02	0.406E+02	0.406E+02	0.406E+02
247	AYEAR	11	16	6	0.398E+02	0.398E+02	0.398E+02	0.398E+02
248	AYEAR	11	17	6	0.390E+02	0.390E+02	0.390E+02	0.390E+02
249	AYEAR	11	18	6	0.383E+02	0.383E+02	0.383E+02	0.383E+02
250	AYEAR	11	19	6	0.376E+02	0.376E+02	0.376E+02	0.376E+02
251	AYEAR	11	20	6	0.369E+02	0.369E+02	0.369E+02	0.369E+02
252	AYEAR	11	21	6	0.351E+02	0.351E+02	0.351E+02	0.351E+02

Table D.3

Initial.out

```
LAYER   MONTH   SOIL TEMP.    WATER CONTENT
    1     6    0.2971E+03    0.8877E-01
    2     6    0.2947E+03    0.8910E-01
    3     6    0.2925E+03    0.8947E-01
    4     6    0.2905E+03    0.8987E-01
    5     6    0.2888E+03    0.9032E-01
    6     6    0.2872E+03    0.9081E-01
    7     6    0.2859E+03    0.9137E-01
    8     6    0.2847E+03    0.9201E-01
    9     6    0.2838E+03    0.9273E-01
   10     6    0.2830E+03    0.9356E-01
   11     6    0.2823E+03    0.9454E-01
   12     6    0.2818E+03    0.9570E-01
   13     6    0.2814E+03    0.9711E-01
   14     6    0.2811E+03    0.9886E-01
   15     6    0.2808E+03    0.1011E+00
   16     6    0.2807E+03    0.1041E+00
   17     6    0.2806E+03    0.1084E+00
   18     6    0.2806E+03    0.1150E+00
   19     6    0.2806E+03    0.8877E-01
   20     6    0.2807E+03    0.9454E-01
   21     6    0.2808E+03    0.5000E+00
   22     6    0.2809E+03    0.5000E+00
```

Table D.4

Kinetic.out

```
    T      LAYER  R1(I,2)   R2(I,2)    RO2(I,2)     WW(I)      TS(I,M)     PH(I,3)    PCO2(I,3)
0.60E+01    1 -.2393E-05 -.7476E-04 -.7125E+01 0.8877E-01 0.2971E+03 0.6764E+01 0.3200E-01
0.60E+01    2 -.1996E-05 -.6103E-04 -.5977E+01 0.8910E-01 0.2947E+03 0.6774E+01 0.3200E-01
0.60E+01    3 -.1746E-05 -.5062E-04 -.5073E+01 0.8947E-01 0.2925E+03 0.6768E+01 0.3200E-01
0.60E+01    4 -.1393E-05 -.4294E-04 -.4365E+01 0.8987E-01 0.2905E+03 0.6809E+01 0.3200E-01
0.60E+01    5 -.1189E-05 -.3697E-04 -.3803E+01 0.9032E-01 0.2888E+03 0.6826E+01 0.3200E-01
0.60E+01    6 -.9751E-06 -.3247E-04 -.3359E+01 0.9081E-01 0.2872E+03 0.6868E+01 0.3200E-01
0.60E+01    7 -.8810E-06 -.2888E-04 -.2997E+01 0.9137E-01 0.2859E+03 0.6873E+01 0.3200E-01
0.60E+01    8 -.8037E-06 -.2611E-04 -.2718E+01 0.9201E-01 0.2847E+03 0.6880E+01 0.3200E-01
0.60E+01    9 -.7399E-06 -.2396E-04 -.2497E+01 0.9273E-01 0.2838E+03 0.6888E+01 0.3200E-01
0.60E+01   10 -.6851E-06 -.2230E-04 -.2325E+01 0.9356E-01 0.2830E+03 0.6900E+01 0.3200E-01
0.60E+01   11 -.6367E-06 -.2103E-04 -.2190E+01 0.9454E-01 0.2823E+03 0.6915E+01 0.3200E-01
0.60E+01   12 -.6045E-06 -.2005E-04 -.2087E+01 0.9570E-01 0.2818E+03 0.6926E+01 0.3200E-01
0.60E+01   13 -.5805E-06 -.1932E-04 -.2010E+01 0.9711E-01 0.2814E+03 0.6937E+01 0.3200E-01
0.60E+01   14 -.5642E-06 -.1879E-04 -.1955E+01 0.9886E-01 0.2811E+03 0.6947E+01 0.3200E-01
0.60E+01   15 -.5553E-06 -.1842E-04 -.1919E+01 0.1011E+00 0.2808E+03 0.6957E+01 0.3200E-01
0.60E+01   16 -.5545E-06 -.1818E-04 -.1901E+01 0.1041E+00 0.2807E+03 0.6966E+01 0.3200E-01
0.60E+01   17 -.5636E-06 -.1805E-04 -.1901E+01 0.1084E+00 0.2806E+03 0.6974E+01 0.3200E-01
0.60E+01   18 -.5876E-06 -.1800E-04 -.1923E+01 0.1150E+00 0.2806E+03 0.6981E+01 0.3200E-01
0.60E+01   19 -.4479E-06 -.1804E-04 -.1786E+01 0.8877E-01 0.2806E+03 0.6987E+01 0.3200E-01
0.60E+01   20 -.4733E-06 -.1813E-04 -.1815E+01 0.9454E-01 0.2807E+03 0.6993E+01 0.3200E-01
0.60E+01   21 -.4394E-05 -.4106E-06 -.4917E+00 0.5000E+00 0.2808E+03 0.6751E+01 0.3200E-01
0.60E+01   22 -.4753E-05 -.6844E-12 -.5265E+00 0.5000E+00 0.2809E+03 0.6721E+01 0.3200E-01
```

Table D.5

Oxygen.out

```
    T      LAYER  TS(I,M)    RO2(I,2)     C(I)
0.60E+01     1 0.2971E+03 -.7125E+01 0.8381E+01
0.60E+01     2 0.2947E+03 -.5977E+01 0.8174E+01
0.60E+01     3 0.2925E+03 -.5073E+01 0.7988E+01
0.60E+01     4 0.2905E+03 -.4365E+01 0.7820E+01
0.60E+01     5 0.2888E+03 -.3803E+01 0.7669E+01
0.60E+01     6 0.2872E+03 -.3359E+01 0.7531E+01
0.60E+01     7 0.2859E+03 -.2997E+01 0.7405E+01
0.60E+01     8 0.2847E+03 -.2718E+01 0.7291E+01
0.60E+01     9 0.2838E+03 -.2497E+01 0.7187E+01
0.60E+01    10 0.2830E+03 -.2325E+01 0.7092E+01
0.60E+01    11 0.2823E+03 -.2190E+01 0.7005E+01
0.60E+01    12 0.2818E+03 -.2087E+01 0.6927E+01
0.60E+01    13 0.2814E+03 -.2010E+01 0.6857E+01
0.60E+01    14 0.2811E+03 -.1955E+01 0.6794E+01
0.60E+01    15 0.2808E+03 -.1919E+01 0.6739E+01
0.60E+01    16 0.2807E+03 -.1901E+01 0.6691E+01
0.60E+01    17 0.2806E+03 -.1901E+01 0.6650E+01
0.60E+01    18 0.2806E+03 -.1923E+01 0.6617E+01
0.60E+01    19 0.2806E+03 -.1786E+01 0.6595E+01
0.60E+01    20 0.2807E+03 -.1815E+01 0.6579E+01
0.60E+01    21 0.2808E+03 -.4917E+00 0.1162E+00
0.60E+01    22 0.2809E+03 -.5265E+00 0.6322E-09
```

Table D.6

Pyrite.out

```
   T       LAYER  R1B(I,2)   R2(I,3)    RT(I,2)  ALPHAP(I,2)  PYR(I,2)  PYR(I,3)
 0.60E+01    1 -0.228E-05 -0.733E-04 -0.756E-04  0.902E+04  0.645E+03  0.647E+03
 0.60E+01    2 -0.190E-05 -0.589E-04 -0.608E-04  0.933E+04  0.646E+03  0.648E+03
 0.60E+01    3 -0.166E-05 -0.481E-04 -0.498E-04  0.960E+04  0.647E+03  0.648E+03
 0.60E+01    4 -0.132E-05 -0.401E-04 -0.414E-04  0.983E+04  0.647E+03  0.648E+03
 0.60E+01    5 -0.113E-05 -0.340E-04 -0.351E-04  0.100E+05  0.647E+03  0.648E+03
 0.60E+01    6 -0.923E-06 -0.293E-04 -0.302E-04  0.102E+05  0.648E+03  0.648E+03
 0.60E+01    7 -0.833E-06 -0.257E-04 -0.266E-04  0.103E+05  0.648E+03  0.648E+03
 0.60E+01    8 -0.759E-06 -0.230E-04 -0.237E-04  0.103E+05  0.648E+03  0.648E+03
 0.60E+01    9 -0.698E-06 -0.208E-04 -0.215E-04  0.104E+05  0.648E+03  0.648E+03
 0.60E+01   10 -0.646E-06 -0.191E-04 -0.198E-04  0.104E+05  0.648E+03  0.648E+03
 0.60E+01   11 -0.600E-06 -0.179E-04 -0.185E-04  0.104E+05  0.648E+03  0.648E+03
 0.60E+01   12 -0.569E-06 -0.169E-04 -0.174E-04  0.104E+05  0.648E+03  0.648E+03
 0.60E+01   13 -0.546E-06 -0.161E-04 -0.166E-04  0.104E+05  0.648E+03  0.648E+03
 0.60E+01   14 -0.530E-06 -0.155E-04 -0.160E-04  0.104E+05  0.648E+03  0.648E+03
 0.60E+01   15 -0.522E-06 -0.151E-04 -0.156E-04  0.104E+05  0.648E+03  0.648E+03
 0.60E+01   16 -0.521E-06 -0.148E-04 -0.153E-04  0.104E+05  0.648E+03  0.648E+03
 0.60E+01   17 -0.529E-06 -0.146E-04 -0.152E-04  0.103E+05  0.648E+03  0.648E+03
 0.60E+01   18 -0.551E-06 -0.145E-04 -0.151E-04  0.103E+05  0.648E+03  0.648E+03
 0.60E+01   19 -0.420E-06 -0.145E-04 -0.150E-04  0.103E+05  0.648E+03  0.648E+03
 0.60E+01   20 -0.444E-06 -0.146E-04 -0.150E-04  0.102E+05  0.648E+03  0.648E+03
 0.60E+01   21 -0.928E-06 -0.260E-06 -0.119E-05  0.135E+05  0.650E+03  0.650E+03
 0.60E+01   22 -0.561E-06 -0.131E-06 -0.692E-06  0.146E+05  0.650E+03  0.650E+03
```

Table D.8
Speciati.out

```
     T          I  CASE(I)   PH(I,2)    PH(I,3)  NPHIT
 0.6000E+01     1   C111  0.6759E+01 0.6764E+01    1
 0.6000E+01     2   C111  0.6768E+01 0.6774E+01    1
 0.6000E+01     3   C111  0.6763E+01 0.6768E+01    1
 0.6000E+01     4   C111  0.6804E+01 0.6809E+01    1
 0.6000E+01     5   C111  0.6822E+01 0.6826E+01    1
 0.6000E+01     6   C111  0.6864E+01 0.6866E+01    1
 0.6000E+01     7   C111  0.6869E+01 0.6873E+01    1
 0.6000E+01     8   C111  0.6876E+01 0.6880E+01    1
 0.6000E+01     9   C111  0.6885E+01 0.6888E+01    1
 0.6000E+01    10   C111  0.6897E+01 0.6900E+01    1
 0.6000E+01    11   C111  0.6912E+01 0.6915E+01    1
 0.6000E+01    12   C111  0.6923E+01 0.6926E+01    1
 0.6000E+01    13   C111  0.6934E+01 0.6937E+01    1
 0.6000E+01    14   C111  0.6944E+01 0.6947E+01    1
 0.6000E+01    15   C111  0.6954E+01 0.6957E+01    1
 0.6000E+01    16   C111  0.6963E+01 0.6966E+01    1
 0.6000E+01    17   C111  0.6971E+01 0.6974E+01    1
 0.6000E+01    18   C111  0.6979E+01 0.6981E+01    1
 0.6000E+01    19   C111  0.6985E+01 0.6987E+01    1
 0.6000E+01    20   C111  0.6991E+01 0.6993E+01    1
 0.6000E+01    21   C112  0.6781E+01 0.6751E+01    1
 0.6000E+01    22   C112  0.6746E+01 0.6721E+01    1
```

Table D.7
Transpor.out

```
     T       I CASE    PH       AFLUX       GYP        ALOH3      FEOH3       ALT        AL3        FE2T       FE3T       FE3        SO4        SO4T        CA        CACO3      POTAS       RPYR       PYR       ATOTAL      AYEAR
0.6000E+01   1 C111 0.6759E+01 0.6857E+00 0.4612E+03 0.6500E+02 0.7264E+02 0.4230E-05 0.1007E-09 0.7555E-04 0.5749E-10 0.1047E-17 0.1539E-01 0.2314E-01 0.6394E-02 0.4551E+01 0.1273E-04 0.6820E+00 0.6454E+03 0.2047E+01 0.2047E+01
0.6000E+01   2 C111 0.6768E+01 0.7447E+00 0.4788E+03 0.6500E+02 0.7242E+02 0.4221E-05 0.9450E-10 0.1381E-03 0.5712E-10 0.9823E-18 0.1605E-01 0.2380E-01 0.6129E-02 0.4816E+01 0.1393E-04 0.5670E+00 0.6461E+03 0.3370E+01 0.3370E+01
0.6000E+01   3 C111 0.6763E+01 0.7092E+00 0.4785E+03 0.6500E+02 0.7227E+02 0.4226E-05 0.9816E-10 0.1799E-03 0.5734E-10 0.1020E-17 0.1565E-01 0.2340E-01 0.6286E-02 0.5012E+01 0.1487E-04 0.4779E+00 0.6466E+03 0.4778E+01 0.4778E+01
0.6000E+01   4 C111 0.6804E+01 0.9848E+00 0.4783E+03 0.6500E+02 0.7215E+02 0.4190E-05 0.7385E-10 0.9036E-03 0.5575E-10 0.7677E-18 0.1892E-01 0.2667E-01 0.5200E-02 0.5161E+01 0.3113E-04 0.4068E+00 0.6470E+03 0.6640E+01 0.6640E+01
0.6000E+01   5 C111 0.6822E+01 0.1114E+01 0.4782E+03 0.6500E+02 0.7207E+02 0.4175E-05 0.6522E-10 0.1401E-02 0.5511E-10 0.6700E-18 0.2056E-01 0.2830E-01 0.4786E-02 0.5264E+01 0.4747E-04 0.3514E+00 0.6473E+03 0.7912E+01 0.7912E+01
0.6000E+01   6 C111 0.6864E+01 0.1443E+01 0.4781E+03 0.6500E+02 0.7202E+02 0.4143E-05 0.4886E-10 0.1754E-02 0.5370E-10 0.5079E-18 0.2492E-01 0.3267E-01 0.3948E-02 0.5330E+01 0.6313E-04 0.3072E+00 0.6475E+03 0.8735E+01 0.8735E+01
0.6000E+01   7 C111 0.6869E+01 0.1485E+01 0.4781E+03 0.6500E+02 0.7198E+02 0.4140E-05 0.4710E-10 0.1881E-02 0.5353E-10 0.4896E-18 0.2554E-01 0.3329E-01 0.3853E-02 0.5367E+01 0.1528E-03 0.2724E+00 0.6476E+03 0.9343E+01 0.9343E+01
0.6000E+01   8 C111 0.6876E+01 0.1546E+01 0.4781E+03 0.6500E+02 0.7196E+02 0.4135E-05 0.4485E-10 0.2026E-02 0.5331E-10 0.4662E-18 0.2638E-01 0.3413E-01 0.3729E-02 0.5394E+01 0.1525E-03 0.2452E+00 0.6477E+03 0.1007E+02 0.1007E+02
0.6000E+01   9 C111 0.6885E+01 0.1625E+01 0.4781E+03 0.6500E+02 0.7194E+02 0.4128E-05 0.4219E-10 0.2189E-02 0.5304E-10 0.4386E-18 0.2748E-01 0.3523E-01 0.3580E-02 0.5409E+01 0.1521E-03 0.2235E+00 0.6478E+03 0.1098E+02 0.1098E+02
0.6000E+01  10 C111 0.6897E+01 0.1734E+01 0.4780E+03 0.6500E+02 0.7194E+02 0.4120E-05 0.3889E-10 0.2406E-02 0.5268E-10 0.4043E-18 0.2902E-01 0.3676E-01 0.3391E-02 0.5415E+01 0.1518E-03 0.2063E+00 0.6478E+03 0.1109E+02 0.1109E+02
0.6000E+01  11 C111 0.6912E+01 0.1883E+01 0.4780E+03 0.6500E+02 0.7194E+02 0.4110E-05 0.3497E-10 0.2674E-02 0.5224E-10 0.3635E-18 0.3115E-01 0.3889E-01 0.3159E-02 0.5414E+01 0.1513E-03 0.1926E+00 0.6478E+03 0.1274E+02 0.1274E+02
0.6000E+01  12 C111 0.6923E+01 0.1995E+01 0.4780E+03 0.6500E+02 0.7194E+02 0.4103E-05 0.3240E-10 0.2885E-02 0.5192E-10 0.3368E-18 0.3277E-01 0.4052E-01 0.3002E-02 0.5408E+01 0.1509E-03 0.1819E+00 0.6478E+03 0.1355E+02 0.1355E+02
0.6000E+01  13 C111 0.6934E+01 0.2110E+01 0.4780E+03 0.6500E+02 0.7194E+02 0.4096E-05 0.3006E-10 0.3102E-02 0.5162E-10 0.3125E-18 0.3445E-01 0.4220E-01 0.2856E-02 0.5398E+01 0.1506E-03 0.1735E+00 0.6478E+03 0.1434E+02 0.1434E+02
0.6000E+01  14 C111 0.6944E+01 0.2225E+01 0.4780E+03 0.6500E+02 0.7195E+02 0.4090E-05 0.2798E-10 0.3322E-02 0.5134E-10 0.2908E-18 0.3614E-01 0.4389E-01 0.2722E-02 0.5386E+01 0.1503E-03 0.1671E+00 0.6478E+03 0.1509E+02 0.1509E+02
0.6000E+01  15 C111 0.6954E+01 0.2337E+01 0.4780E+03 0.6500E+02 0.7196E+02 0.4084E-05 0.2615E-10 0.3541E-02 0.5109E-10 0.2719E-18 0.3780E-01 0.4555E-01 0.2603E-02 0.5372E+01 0.1500E-03 0.1623E+00 0.6478E+03 0.1580E+02 0.1580E+02
0.6000E+01  16 C111 0.6963E+01 0.2444E+01 0.4780E+03 0.6500E+02 0.7197E+02 0.4079E-05 0.2458E-10 0.3755E-02 0.5086E-10 0.2555E-18 0.3940E-01 0.4715E-01 0.2497E-02 0.5356E+01 0.1497E-03 0.1589E+00 0.6478E+03 0.1646E+02 0.1646E+02
0.6000E+01  17 C111 0.6971E+01 0.2544E+01 0.4780E+03 0.6500E+02 0.7198E+02 0.4074E-05 0.2324E-10 0.3961E-02 0.5065E-10 0.2416E-18 0.4090E-01 0.4865E-01 0.2406E-02 0.5340E+01 0.1495E-03 0.1566E+00 0.6477E+03 0.1706E+02 0.1706E+02
0.6000E+01  18 C111 0.6979E+01 0.2637E+01 0.4780E+03 0.6500E+02 0.7199E+02 0.4070E-05 0.2209E-10 0.4157E-02 0.5047E-10 0.2297E-18 0.4230E-01 0.5005E-01 0.2326E-02 0.5322E+01 0.1493E-03 0.1553E+00 0.6477E+03 0.1760E+02 0.1760E+02
0.6000E+01  19 C111 0.6985E+01 0.2721E+01 0.4780E+03 0.6500E+02 0.7200E+02 0.4067E-05 0.2114E-10 0.4340E-02 0.5031E-10 0.2197E-18 0.4357E-01 0.5132E-01 0.2258E-02 0.5314E+01 0.1491E-03 0.1537E+00 0.6477E+03 0.1808E+02 0.1808E+02
0.6000E+01  20 C111 0.6991E+01 0.2797E+01 0.4780E+03 0.6500E+02 0.7201E+02 0.4064E-05 0.2032E-10 0.4510E-02 0.5018E-10 0.2112E-18 0.4473E-01 0.5248E-01 0.2200E-02 0.5296E+01 0.1489E-03 0.1539E+00 0.6476E+03 0.1850E+02 0.1850E+02
0.6000E+01  21 C112 0.6781E+01 0.2625E+01 0.4779E+03 0.6500E+02 0.7123E+02 0.4663E-05 0.9553E-10 0.4606E-02 0.5660E-10 0.8965E-18 0.4403E-01 0.5178E-01 0.2235E-02 0.6243E+01 0.1491E-03 0.1601E-01 0.6495E+03 0.1732E+02 0.1732E+02
0.6000E+01  22 C112 0.6746E+01 0.2809E+00 0.4765E+03 0.6500E+02 0.7117E+02 0.4626E-05 0.1197E-09 0.2625E-02 0.5801E-10 0.1141E-17 0.2534E-01 0.3309E-01 0.3883E-02 0.6383E+01 0.8706E-04 0.1010E-01 0.6497E+03 0.1732E+01 0.1732E+01
```

APPENDIX E

INPUT PARAMETER DESCRIPTIONS

Model Symbol	Parameter Description	Units	Nominal Value	Probabilistic Distribution	Computer Symbol	Old Computer Symbol
1. INITIAL INVENTORY MODEL						
A_o	emperical temperature coefficient	°K	20	C(20)	COEFAO	AO
Cover	nontailings material	m	0	C(0)	COVER	COVER
d	dampening depth	m	2.0	C(2.0)	COEFDD	D
h_e*	air entry value	m	-0.5	T(-1.5,-0.5,-0.05)	HE(i)	HE(i)
L	phase shift constant	unitless	0.1	C(0.1)	COEFPS	COEF
n_r*	residual water content	$m_w^3 \cdot m_{tail}^{-3}$	0.08	N(0.08,0.01, 0.05,0.11)	NR(i)	NR(i)
N_t*	porosity	$m_{void}^3 \cdot m_{tail}^{-3}$	0.50	T(0.45,0.50,0.55)	NT(i)	NT(i)
t	bulk density of the tailings	$kg.m^{-3}$	1.3E6	C(1.3E6)	BULKD	BD
T_m	yearly mean temperature	°K	283	C(283)	AVGTEM	TAVG
X_{pyr}	mass fraction of pyrite	$g.g^{-1}$	0.06	U(0.048,0.072)	XPYR	XPYR
X_{gyp}	mass fraction of gypsum	$g.g^{-1}$	0.05	U(0.04,0.06)	XGYP	XGYP
X_{FeOOH}	mass fraction of ferric hydroxide	$g.g^{-1}$	0.0041	U(0.0025,0.0057)	XFEOH3	XFEOH3
X_{ALOH3}	mass fraction of basaluminate	$g.g^{-1}$	0.0023	U(0.0014,0.0032)	XALOH3	XALOH3
X_{ser}	mass fraction of sericite	$g.g^{-1}$	0.136	U(0.11,0.16)	XSER	XSER
X_{cal}	mass fraction of calcite	$g.g^{-1}$	0.0005	U(0.000,0.001)	XCACO3	XCACO3
λ*	soil coefficient for moisture content	unitless	0.73	U(0.68,0.78)	LA(i)	LA(i)
ϕ	fraction of water migrating from mixing to deep zones	unitless	0.20	C(0.20)	VRFRAC	

Continued

Model Symbol	Parameter Description	Units	Nominal Value	Probabilistic Distribution	Computer Symbol	Old Computer Symbol
2. KINETICS MODULE						
E_a	biological energy of activation	$cal.mol^{-1}$	11,700	T(10000,11700, 16300)	BIOEA	EA1
E_{ac}	chemical energy of activation	$cal.mol^{-1}$	13,300	C(13300)	CHEMEA	EA2
K_c	chemical rate constant	$mol.m^{-2}.month^{-1}.atm$	$2.3x10^6$	$T(1.18x10^5,2.36x10^6, 4.72x10^7)$	CHEMKC	KCONST
L_p	limiting phosphorus concentration	$mol.m^{-3}$	$1.29x10^{-3}$	$C(1.29x10^{-3})$	LIMP	LP
μ_{max}	maximum specific growth rate	mth^{-1}	13.0	U(11.5,14.5)	BIOMAX	UMAX
X_p	biomass per surface area of pyrite	$g.m^{-2}$	$1.6x10^{-3}$	$LN(1.6x10^{-3}, 1.7,3.2x10^{-4}, 7.8x10^{-3})$	BIOXP	XP
$Y_{x/s}$	biomass yield constant	$g.mol^{-1}$	3.2	T(2.5,3.2,4.2)	BIOYXS	YXS
3. OXYGEN TRANSPORT MODULE						
dx*	thickness of each layer	m	0.20	C(0.20)	DX(i)	DX(i)
L_t	number of layers	unitless	22	C(22)	LAYER	L
L_s	first layer of saturated zone	unitless	21	C(21)	LAYSAT	LS
H	Henry's Law constant for oxygen	unitless	23.6	C(23.6)	HENRY	HENRY
Z	depth of water table	m	4.0	C(4.0)	WATTAB	ZWATER
4. PYRITE OXIDATION MODULE						
L_o	limiting oxygen concentration	atm	0.01	C(0.01)	LIMO2	LO2
ρ	molar density of pyrite	$mol.m^{-3}$	41670	C(41670)	MOLARD	OP
r_m	maximum radius	m	$1.25x10^{-4}$	$C(1.25x10^{-4})$	RADMAX	RMAX

Continued

Model Symbol	Parameter Description	Units	Nominal Value	Probabilistic Distribution	Computer Symbol	Old Computer Symbol
X	parentto coefficient	unitless	2	C(2)	COEFX	X
Y	parentto coefficient	unitless	-1	C(-1)	COEFY	Y
α	emperical parameter for particle distribution	unitless	0.9	C(0.9)	ALPHA	AL
β	emperical parameter for particle distribution	unitless	1.8	C(1.8)	BETA	BE

5. SOLUTE TRANSPORT MODULE

Model Symbol	Parameter Description	Units	Nominal Value	Probabilistic Distribution	Computer Symbol	Old Computer Symbol
A_x	area of tailings	m^2	$3.0x10^7$	$C(3.0x10^7)$	ATAIL	ATAIL
Vr	infiltration rate for each month (i.e. for January,m=1; June,m=6)	$m.mth^{-1}$	m=1, 0.005	T(0.001,0.005,0.01)	VR(m)	VRI(m)
			m=2, 0.005	T(0.001,0.005,0.01)		
			m=3, 0.005	T(0.001,0.005,0.01)		
			m=4, 0.090	T(0.018,0.09,0.18)		
			m=5, 0.070	T(0.014,0.07,0.14)		
			m=6, 0.030	T(0.006,0.03,0.06)		
			m=7, 0.020	T(0.004,0.02,0.04)		
			m=8, 0.030	T(0.006,0.03,0.06)		
			m=9, 0.050	T(0.01,0.05,0.1)		
			m=10, 0.050	T(0.01,0.05,0.1)		
			m=11, 0.040	T(0.008,0.04,0.08)		
			m=12, 0.005	T(0.001,0.005,0.01)		

6. AQUEOUS SPECIATION MODULE

Model Symbol	Parameter Description	Units	Nominal Value	Probabilistic Distribution	Computer Symbol	Old Computer Symbol
f_{ALOH}	emperical coefficient for aluminum convergence	unitless	0.075	T(0.01,0.075,0.6)	COEFAL	FALOH
CHSO4	T.S. constant for HSO_4	$(mol.L^{-1})^{-1}$	$1.26x10^{-2}$	$C(1.26x10^{-2})$	CHSO4	CHSO4
CCASO4	T.S. constant for $CASO_4$	$(mol.L^{-1})^{-1}$	316.23	C(316.23)	CCASO4	CCASO4
CALSO4	T.S. constant for $ALSO_4$	$(mol.L^{-1})^{-1}$	1047.13	C(1047.13)	CALSO4	CALSO4
CFEOH	T.S. constant for FEOH	$(mol.L^{-1})^{-1}$	$6.46x10^{-3}$	$C(6.46x10^{-3})$	CFEOH	CFEOH

Continued

Model Symbol	Parameter Description	Units	Nominal Value	Probabilistic Distribution	Computer Symbol	Old Computer Symbol
7. OUTPUT FLAGS						
flag1	output control flag for initial module		1	C(1)	FLAG1	
flag2	output control flag for kinetic module		1	C(1)	FLAG2	
flag3	output control flag for oxygen module		1	C(1)	FLAG3	
flag4	output control flag for pyrite module		1	C(1)	FLAG4	
flag5	output control flag for transport module		1	C(1)	FLAG5	
flag6	output control flag for speciation module		1	C(1)	FLAG6	
month	output control flag to specify which month output is required for		6	C(6)	MONTH	

Key to Probability Distributions:

C - Constant (single value)
T - Triangular (min., mode, max)
U - Uniform (min., max)
LN - Lognormal (geo. mean, geo. std. dev., min., max.)
N - Normal (mean, std.dev., min., max.)

Notes
T.S. = thermodynamic stability constants
C.B. = charge balance equation
* = input parameters are required for each layer

APPENDIX F

INTERMEDIATE PARAMETERS

CALCULATED PARAMETERS

Model Symbol	Parameter Description	Units	Origin	Computer Symbol
AFLUX	acid flux	mol.m^{-2}	TRANSPORT	AFLUX
Al^{3+}	aqueous aluminum concentration	mol.L^{-1}	TRANSPORT	AL3(i,t)
$Al(OH)_3$	aluminum solids	mol.m^{-3}	TRANSPORT	ALOH3(i,t)
α_p	surface area of pyrite per unit volume of tailings	m^2.m^3	PYRITE	ALPHAP(i,t)
Al_T	total aqueous aluminum concentration	mol.L^{-1}	TRANSPORT	ALT(i,t)
ALUM	aluminum species present in C.B.eq.	mol.L^{-1}	SPECIATION	ALUM(i,t)
As	surface area of pyrite	m^2	PYRITE	AS(i,t)
ATOTAL	accumulated acid flux for test period	mol.m^{-2}	TRANSPORT	ATOTAL
AYEAR	accumulated acid flux for calendar year	mol.m^{-2}	TRANSPORT	AYEAR
C	oxygen concentration in air phase	mol.m^{-3}	OXYGEN	C(i)
Ca^{2+}	calcium concentration	mol.L^{-1}	OXYGEN	CA(i,t)
Co	initial oxygen concentration in air phase at surface	mol.m^{-3}	OXYGEN	CO
Ck	kinetics constant	unitless	KINETICS	CONST
C	oxygen concentration in air phase	mol.m^3	OXYGEN	COX(i,t)
C_T	total inorganic carbon	mol.L^{-1}	TRANSPORT	CT(i,t)
C_w	oxygen concentration in porewater	mol.m^{-3}	OXYGEN	CW(i)
De	effective diffusivity through tailings	m^2.mth^{-1}	OXYGEN	DE(i,t)

Continued,

Model Symbol	Parameter Description	Units	Origin	Computer Symbol
Fe^{2+}	ferrous iron concentration	$mol.L^{-1}$	TRANSPORT	FE2(i,t)
Fe^{3+}	ferric iron concentration	$mol.L^{-1}$	TRANSPORT	FE3(i,t)
$Fe(OH)_3$	iron solids	$mol.m^{-3}$	TRANSPORT	FEOH3(i,t)
fp	pH dependence factor	unitless	KINETIC	FPH
h	height above the water table	m	INITIAL	H(i)
HCO_3	carbonate concentration	$mol.L^{-1}$	TRANSPORT	HCO3(i,t)
H^+	hydrogen ion concentration	$mol.L^{-1}$	SPECIATION	HI(i,t)
V	infiltration rate of water into the tailings	$m.mth^{-1}$	INITIAL	INFILT(i,m)
IRON3	ferric iron species present in C.B.eq.	$mol.L^{-1}$	SPECIATION	IRON(i,t)
Ko	rate constant	$m.mth^{-1}$	PYRITE	K(i,t)
Kb	bulk oxygen reaction rate constant	mth^{-1}	OXYGEN	KB(i)
Lc	first layer of the capillary fringe	unitless	INITIAL	LC
n_a	volumetric air content of soil	$m^3_{air}.m^{-3}_{tail}$	INITIAL	NA(i)
Np	amount of pyrite	mol	PYRITE	NP(i,t)
n_w	water content	$m^3_w.m^{-3}_{tail}$	INITIAL	NW(i)
P_{CO2}	partial pressure of carbon dioxide	atm	SPECIATION	PCO2(i,t)
pH	measure of hydrogen ion concentration	unitless	SPECIATION	PH(i,t)
P_{O2}	partial pressure of oxygen	atm	OXYGEN	PO2(i,t)

Continued,

Model Symbol	Parameter Description	Units	Origin	Computer Symbol
M	amount of pyrite per unit volume of tailings	mol.m^{-3}	PYRITE	PYR(i,t)
R_{02}	rate of oxygen depletion	mol.m^{2}.mth^{-1}	KINETIC	R(i,t)
R_1	specific rate of biological reaction	mol.m^{-2}.mth^{-1}	KINETIC	RI(i,t)
R_{1b}	oxygen influenced biological specific reaction rate	mol.m^{-2}.mth^{-1}	PYRITE	R1B(i,t)
R_2	specific rate of chemical reaction	mol.m^{-2}.mth^{-1}	KINETIC	R2(i,t)
RO_2	rate of oxygen depletion	mol.m^{-2}.mth^{-1}	KINETIC	RO2(i,t)
R_{pyr}	overall reaction rate per volume of tailings	mol.m^{-3}.mth^{-1}	PYRITE	RPYR(i,t)
R_t	overall specific reaction rate	mol.m^{-2}.mth^{-1}	PYRITE	RT(i,t)
S	water saturation	m^3.m^{-3}	KINETIC	S(i)
SO_4	sulphate concentration	mol.L^{-1}	TRANSPORT	SO4(i,t)
S_T	total dissolved sulphates	mol.L^{-1}	TRANSPORT	SO4T(i,t)
SULF	sulphate species present in C.B.eq.	mol.L^{-1}	SPECIATION	SULF(i,t)
T_s	soil monthly temperature	°K	INITIAL	TS(i,m)
μ	specific growth rate	mth^{-1}	KINETIC	U(i,t)
U	ratio of oxygen reaction rate to diffusivity	m^{-1}	OXYGEN	UR(i,t)
q	infiltration rate	L.mth^{-1}	INITIAL	VRAIN(im,)
V_t	volume of layer	m^3	INITIAL	VT(i)
X	actual depth of a layer	m	INITIAL	Z(i)

APPENDIX G

ERROR AND WARNING MESSAGES

APPENDIX G

ERROR AND WARNING MESSAGES

(003) ERROR IN INPUT FILE

An error occured reading the indicated line of the input file. Check all counters and the format of inputs on the line of the error.

(004) CORRELATED NAME NOT FOUND

Name of independent variable for correlated distribution not found in input file. Distribution name must appear before correlated parameter.

(005) UNEXPECTED END OF DATA

Input file empty, doesn't exist, or too short.

(006) TYPE ERROR IN REGULAR DIST'ns

Distribution type number greater than 8. Numbers of parameters or arbitrary or correlated distributions incorrect.

(007) TYPE ERROR IN CORRELATED DIST'ns

Distribution type number not equal to 10. Numbers of parameters or arbitrary or correlated distributions incorrect.

(008) TYPE ERROR IN ARBITRARY DIST'ns

Distrubtion type number not equal to 9. Numbers of parameters or arbitrary or correlated distributions incorrect.

(009) NUMBER OF PARAMETERS INCORRECT

End of file reached before specified numbers of parameters read.

(011) TIME STEPS MUST INCREASE

Months to be saved for output must increase.

(012) DISTRIBUTION NUMBER NOT DEFINED

(018) CANNOT CORRELATE PARAMETERS

The independent parameter cannot be time variant unless the dependent parameter is.

(028) TOO MANY OUTPUTS

A maximum of 300 variables can be output to the detailed results and key files. Reduce number of variables or number of time steps.

(029) FILE NOT FOUND

Input file named does not exist.

(030) ERROR IN LOGNORMAL SPECIFIERS

Lognormal distribution has equal, reversed, or undefined minimum and maximum values. Check input file.

(031) ERROR IN NORMAL SPECIFIERS

Normal distributions has equal, reversed, or undefined minimum and maximum values. Check input file.

(032) TIME MUST BE IN WHOLE NUMBERS

The simulation time must correspond to the time step, namely, one month.

(033) ERROR IN TRIANGULAR SPECIFIERS

Triangular distribution has equal, reversed, or undefined minimum and maximum values. Check input file.

(034) ERROR IN BETA SPECIFIERS

Either the minimum is greater than or equal to the maximum specified or A or B are not greater than zero.

(050) ERROR IN THE VALUE INPUT FOR WATTAB, DX OR LAYSAT

Indicates inconsistent values input for WATTAB, LAYSAT, or DX. Check input files.

(051) UNACCEPTABLE NUMBER OF LAYERS

Indicates value of layer is too large. Maximum accepted is 22.

(052) CALCULATED pH LESS THAN ZERO

Program has calculated a value for pH that is less than zero.

(053) MAXIMUM NUMBER OF ITERATIONS HAS BEEN EXCEEDED

Maximum number of iterations allowed for solving the pH equation has been exceeded.

(102) ABOUT TO OVER WRITE EXISTING FILE

Continuing execution will cause the contents of the file named directly above the warning to be erased.